

# SHOCK WAVE STRUCTURE IN BINARY GAS MIXTURE

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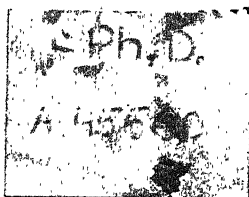
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DEPARTMENT OF MECHANICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

JUNE ~~MAY~~ 1974



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# SHOCK WAVE STRUCTURE IN BINARY GAS MIXTURE

A Thesis Submitted  
In Partial Fulfilment of the Requirements  
for the Degree of  
DOCTOR OF PHILOSOPHY

By  
U. N. SINHA

to the

DEPARTMENT OF MECHANICAL ENGINEERING  
INDIAN INSTITUTE OF TECHNOLOGY KANPUR  
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CERTIFICATE:

Certified that this work has been carried out  
under my supervision and that this has not been  
submitted elsewhere for a degree.

  
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Uday Narayan Sinha

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## List of Important Symbols

$\mathbf{c}$	-	Molecular Velocity of a particle
$c_p$	-	Specific Heat at constant pressure
$\mathbf{C}$	-	Peculiar Velocity of a molecule
$f$	-	One-particle distribution function
$\mathbf{F}$	-	Force acting on a particle of unit mass
$F_2$	-	Two-particle distribution function
$\mathbf{g}$	-	Relative velocity of second molecule with respect to <del>second</del> first molecule
$J$	-	Collision integral
$k$	-	Boltzmann constant
$K_{ij}$	-	Constant of proportionality of force field of interaction between two particles
$L$	-	Length Scale
$m$	-	mass of a particle
$M$	-	Mach Number
$n$	-	Number of particles per unit volume of

physical space - Number Density

$N^-, N^+$  - Upstream and down stream (respectively) number density terms corresponding to the Bimodal description of Mott-Smith

$P_{ij}$  - Stress Tensor

$\vec{q}$  - Heat flux vector

$R$  - Characteristic gas constant

$t$  - Time

$T$  - Temperature

$T^-, T^+$  - Upstream and downstream (respectively) temperatures corresponding to the Bimodal description of Mott-Smith

$\vec{u}$  - Mean velocity of the molecules

$U^-, U^+$  - Upstream and downstream (respectively) mean molecular velocities corresponding to the Bimodal description of Mott-Smith

$x$  - Position coordinate of a particle

$$x_{12} = \left( \frac{m_1 + m_2}{2m_2} - \frac{K_{12}}{K_{11}} \right)^{\frac{1}{2}} = 1.385 \text{ (He-Ar PAIR) UNLESS OTHERWISE}$$

$$x_{22} = \left( \frac{m_1}{m_2} - \frac{K_{22}}{K_{11}} \right)^{\frac{1}{2}} = 0.88 \text{ (He-Ar PAIR)}$$

$\alpha$  - Concentration ratio

$\beta$  - Mass ratio

$\epsilon$  - Ratio of the velocities across the Shock

$\sigma$  - Molecular diameter =  $15 \text{ (He-Ar PAIR)}$

$\Omega$  - Solid angle

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## SYNOPSIS

A numerical analysis of steady, normal shock wave structure in binary gas mixtures of inert, monatomic gases is made. The analysis is based on the moment method of kinetic theory coupled with Mott-Smith ansatz.. The governing equations of this two temperature- two velocity model are in no way restricted by initial concentration of the species, mass ratio of the species or Mach number. The system of equations which describes the structure includes the conservation of mass of each species, the conservation of momentum and energy of the mixture and two transfer equations. The non dimensional parameters which appear are the mass ratio, free stream Mach number and initial concentration ratio.

Only the rigid sphere gas and the Maxwell molecule have been examined to study the effect of molecular model on the structure. Regarding the transfer equation, the choice had been dictated by simplicity and is either  $C_x^2$  or  $C_x^3$  moment of Boltzmann equation where  $C_x$  is the velocity of the particle in the x-direction. For particular cases, a given type of structure suggests more than one scale for a complete transition. Comparison with existing experimental and theoretical results is made.

The governing equations form a system of two coupled, nonlinear, autonomous, ordinary differential equations whose boundary and regularity conditions are prescribed at the two infinities. This has been reduced to an initial value problem by analysing the singular points in the phase plane of the system and the existence and uniqueness of the solution have been considered.

Finally, the arbitrariness of moment method has been discussed and a criterion to remove the arbitrariness has been suggested. For a special case of Mach number tending to infinity and rigid sphere gas numerical result has been presented which is nearest to the true Boltzmann solution in  $L_2$  norm when the assumed representation of the distribution function is bimodal.

## **INTRODUCTION**



## INTRODUCTION.

The problem of the structure of a shock wave is one of the classical problems in the sense that it is conceptually simple, physically important and has no boundaries - boundary conditions are put at  $\pm \infty$ ; still it is a challenging problem.

The equations of conservation of mass, momentum and energy for a one dimensional steady flow of an ideal gas admit a non-trivial solution which represents a possible jump in the flow quantities like velocity, temperature, pressure, entropy etc provided the upstream Mach number is greater than one. In this hydrodynamic description, shock wave is a plane of discontinuity. Jump in entropy indicates a dissipation of mechanical energy and an irreversible conversion of mechanical energy into heat.

The consideration of steady, one dimensional flow of a viscous, heat conducting fluid, approaching finite limit values at  $x = -\infty$  and  $x = +\infty$  (these limiting values being interrelated) includes the two dissipating mechanisms viz. viscosity and heat conduction attributable to the molecular structure of the fluid. These mechanisms account for the irreversible transfer of

mechanical energy into heat and replace the plane of discontinuity in the flow variable by a thin layer, sometimes called the shock layer in which steep gradients appear. It is believed that the two dissipative mechanisms play entirely different roles. Viscous mechanism causes the scattering of the directed momentum of the incident gas and the conversion of the kinetic energy of the directed molecular motion into the kinetic energy of the random motion. Role of the heat conduction is secondary in as much as it indirectly affects the conversion of the mechanical energy as a result of redistribution of pressure. (Zel'dovich and Raizer (1967)).

The solution of the one dimensional hydrodynamic equations neglecting viscosity but retaining heat conduction was ~~studied~~ studied by Rayleigh (1910) who proved that a continuous solution for the flow variable is possible only for weak shocks. On the other hand, continuous solution of all flow parameters for all shock strengths exists by considering viscosity even if heat conduction is neglected. Qualitatively, the problem is studied by Rayleigh, Weyl (1949) and Gilbarg (1951). For a fairly general set of perfect gases for which a relation among coefficient of viscosity, thermal conductivity and specific heat at constant pressure is postulated,

explicit integrations of the equations of motion has been carried out. (Becker (1922), Puckett and Stewart (1950), Morduchow and Libby (1949)).

As the characteristic length scale of the shock layer is the mean free path, the question of appropriateness of continuum and kinetic description arises naturally. The Navier-Stokes equations provide a solution of the shock structure for any strength of the shock where as the Burnett equations fail to give a shock structure for an upstream Mach number above 2.2 as found by Zoller (1951). This, along with the experimental work of Sherman and Talbot (1960), led to a wide spread use of the Navier-Stokes theory for the study of the shock wave structure, with <sup>-out</sup> elaborating restrictions on the Mach number. However, except for low Mach number, the agreement between the Navier-Stokes results and experimental results is not very satisfactory. Hence, though one may admit (██████████) (██████████) adequacy of the Navier-Stokes theory for low Mach numbers, in general, it is untenable to think of any continuum theory as appropriate for a situation in which the mean free path is a significant fraction of the shock thickness, the only macroscopic length relevant to the problem. Consequently attempts have been made to examine the structure of the shock wave from the kinetic theory point of view using the Boltzmann equations.

The study of the shock structure may, at first sight, appear to be of academic interest only in as much as the downstream conditions can be obtained without determining its structure and its thickness is very small. In fact, to the order of quantities studied in the classical shock structure, its knowledge throws some light on the physical nature of the shock wave. One field where the knowledge of shock structure may have a direct application is the study of flames. However, when the global problem for flow past an obstacle is studied along with the higher order effects (for a curved shock wave), the knowledge of the shock structure becomes a necessity to know the modified Rankine Hugoniot conditions. In the case of corresponding mixture problem, the concentration ratio gets modified which cannot be determined without knowing the shock structure (Oberai (1965)).

#### Boltzmann Equation:

The governing equation for non-uniform flow of a single gas in terms of one particle distribution function is the Boltzmann equation.

$$\begin{aligned} \frac{Df}{Dt} &\equiv \frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{c}} = J(f, f) \\ &\equiv \int (f' f_1' - f f_1) g \, d\Omega \, d\mathbf{c}_1 \end{aligned} \quad (0.1)$$

where  $\underline{c}$ ,  $\underline{c}_1$  are the velocities of colliding pair of molecules before collision and  $\underline{c}'$ ,  $\underline{c}_1'$  are their velocities after collision, and where

$$f_1 = f(t, \underline{x}, \underline{c}_1)$$

$$f' = f(t, \underline{x}, \underline{c}')$$

$$f_1' = f(t, \underline{x}, \underline{c}_1')$$

$$\underline{g} = \underline{c}_1 - \underline{c}$$

$$\underline{g}' = \underline{c}_1' - \underline{c}'$$

and  $d\Omega = b db d\phi$  (see fig. 1)

provided

(a) The consideration is restricted to binary collisions - i.e., dilute gas

$$(b) F_2(t, \underline{x}_1, \underline{c}_1, \underline{x}_2, \underline{c}_2) = f(t, \underline{x}_1, \underline{c}_1) f(t, \underline{x}_2, \underline{c}_2)$$

where  $F_2(t, \underline{x}_1, \underline{c}_1, \underline{x}_2, \underline{c}_2)$  is the probability of simultaneously observing 2 molecules in the state  $(\underline{x}_1, \underline{c}_1, \underline{x}_2, \underline{c}_2)$ .

(This is known as postulate of molecular chaos)

and finally

(c) The collision between the pairs of molecules of arbitrary impact parameters  $b$ , are equally probable, i.e., the function  $f(t, \underline{x}_1, \underline{c}_1)$  does not change over distances of the order of the collision cross section.

The validity of the Boltzmann equation is considered by authors like Yvon (1935), Bogolyubov (1946), Born and Green (1946), Kirkwood (1947) and Grad (1958).

From the definition of  $f$ , the number density  $n$  is equal to

$$n(t, \underline{x}) = \int f(t, \underline{x}, \underline{c}) d\underline{c} \quad (0.2)$$

where the integration is performed over all molecular velocities. Similarly, the mean velocity of the molecules, the stress tensor and the energy flux are defined by the relations

$$\underline{u}(t, \underline{x}) = \frac{1}{n} \int \underline{c} f(t, \underline{x}, \underline{c}) d\underline{c} \quad (0.3)$$

$$p_{ij} = m \int c_j c_i f(t, \underline{x}, \underline{c}) d\underline{c} \quad (0.4)$$

$$q_i = \frac{m}{2} \int c^2 c_i f(t, \underline{x}, \underline{c}) d\underline{c} \quad (0.5)$$

Here  $\underline{c} = \underline{c} - \underline{u}$  is the thermal or peculiar velocity of a molecule.

Temperature is identified as the mean energy of thermal motion by the relation

$$\frac{3}{2} kT = \frac{1}{n} \int \frac{m c^2}{2} f(t, \underline{x}, \underline{c}) d\underline{c} \quad (0.6)$$

where  $k$  is the Boltzmann constant.

### Methods in Kinetic Theory to solve the problem of Shock Structure.

Let the  $x$  - axis be directed along the flow. Let  $U_u, N_u, T_u$  and  $U_d^*, N_d^*, T_d^*$  be the mean velocity, density and temperature of the gas, respectively in front of and behind the shock wave.

The gas is in equilibrium at infinity in both

directions (i.e. before and after the shock), therefore, the corresponding distribution functions are Maxwellian:

$$f(x \rightarrow -\infty) = f_1(q) = N_u^{-3/2} (2\pi RT_u) \exp \left[ -\frac{(q - \frac{1}{2} U_u)^2}{2RT_u} \right] \quad (0.7a)$$

$$f(x \rightarrow +\infty) = f_2(q) = N_d^{*-3/2} (2\pi RT_d^*) \exp \left[ -\frac{(q - U_d^*)^2}{2RT_d^*} \right] \quad (0.7b)$$

The investigation of the structure of the shock wave requires the solution of equation (0.1) with the boundary conditions 0.7(a) and 0.7(b) where given  $U_u, T_u, N_u$  the determination of  $N_d^*, U_d^*$  and  $T_d^*$  is a part of the problem.

There is as yet no exact solution for this problem. Monte Carlo trials have been made by Bird (1968) in which a mathematical simulation of the phenomenon is carried out on high speed computer. The molecular model and the collision dynamics are assumed and the motion of one or several of the chosen particles is traced by the computer. Such methods, whatever their merit, are limited by the storage capacity of the computer.

Chorin (1972) has presented a numerical solution of the problem recently. The method takes formidable time on the computer, needs large storage capacity and places particularly heavy demands on the accuracy of the algorithm used.

Model equations instead of the Boltzmann equation have also been solved to throw light on the problem. In these procedures, the collision term of the Boltzmann equation is replaced by suitable simpler expression such that the gross features of collision terms are retained. A well known model is the Krook's model (1954) and the corresponding problem has been solved numerically by Liepmann, Narasimha and Chahine (1962). The success of their method is not restricted by the value of the upstream Mach number. It seems that for strong shocks the upstream side is much smoother than is predicted by Navier-Stokes theory, but it is not known exactly whether it is a property of the Krook equation or happens as well for the full Boltzmann equation.

First satisfactory, approximate solution in analytic form was given by Mott-Smith (1951) for all Mach numbers. He postulates an appropriate form for  $f$ , containing a certain number of parameters (which may be constant or function of  $x$ ). These parameters are determined by taking suitable moments of the Boltzmann equation. The distribution function, according to his postulate, is of the following form:

$$f(x, \underline{c}) = N^*(x) (2\pi RT)^{-\frac{3}{2}} \exp \left[ -\frac{(\underline{c} - \underline{U}_1)^2}{2RT} \right]$$



$$+ N^+(x) (2 \pi R T^*)^{-\frac{3}{2}} \exp \left[ - \frac{(c - U^*)^2}{2 R T^*} \right] \quad (0.8a)$$

with the boundary conditions

$$\lim_{x \rightarrow -\infty} N^-(x) = N_0, \quad \lim_{x \rightarrow -\infty} N^+(x) = 0 \quad (0.8b)$$

The quantities  $U$  and  $T$  are respectively the upstream velocity and temperature. The four unknowns  $N^-(x)$ ,  $N^+(x)$ ,  $U^*$  and  $T^*$  are determined with the help of three conservation equations (viz. mass, momentum and energy) and one (arbitrary) moment equation. The final answer will depend upon the particular extra moment chosen and the molecular model assumed. Despite these limitations, Holway (1963) while examining the effect of collision models upon the shock wave concludes that the Mott-Smith solution is a much better approximation to the solution of the Boltzmann equation than that of the Krook kinetic equation. The numerical computation by Chorin (1972) also lends credence to the results of the Mott-Smith theory. The bimodal character of the distribution function is also confirmed by the calculations of Bird. Salwen et al (1964) attempted to improve the Mott-Smith solution by taking multimodal distribution. It may be mentioned here that the ratio  $\frac{U^*}{U}$  being constant is an essential feature of Mott-Smith ansatz (for the single gas case) and we shall refer to it in the mixture problem.

As far as the problem of shock wave structure in gaseous mixture is concerned, motivated by the success of Mott-Smith theory, its simple extension to the case of gaseous mixture was first given by Oberai (1965). (Fujimoto (1965) also attempted the solution independently but he did not consider the conservation of momentum and energy in the shock and consequently his results appeared to be unrealistic.) Oberai (1965) had given the governing equations for shock wave in a gaseous mixture but he presented solutions only for small concentration ratio. The governing equations are the following.

$$f_i = (x, c) = n_i(x) (2\pi R_i T)^{-3/2} \exp \left\{ - \frac{(c - U_i)^2}{2R_i T} \right\} \\ + n_i^+(x) (2\pi R_i T^*)^{-3/2} \exp \left\{ - \frac{(c - U_i^*)^2}{2R_i T^*} \right\} \\ i = 1, 2 \quad (0.9)$$

$f_i$ 's are the distribution functions for different species.

Writing  $n_i^-(x) = N_0 N_i^-(x)$  and

$$n_i^+(x) = N_0 \frac{U}{U^*} N_i^+(x)$$

$$\frac{dN_i^-(x)}{d\xi} + \frac{dN_i^+(x)}{d\xi} = 0, \quad i = 1, 2 \quad (0.10)$$

$$m_1 \left\{ (U^2 + R_1 T) - (U^{*2} + R_1 T^*) \frac{U}{U^*} \right\} \frac{dN_1}{d\xi} +$$

$$m_2 \left\{ (U^2 + R_2 T) - (U^{*2} + R_2 T^*) \frac{U}{U^*} \right\} \frac{dN_2}{d\xi} = 0 \quad (0.11)$$

$$m_1 \left\{ U(U^2 + 5R_1 T) - U^*(U^{*2} + 5R_1 T^*) \frac{U}{U^*} \right\} \frac{dN_1}{d\xi} +$$

$$m_2 \left\{ U(U^2 + 5R_2 T) - U^*(U^{*2} + 5R_2 T^*) \frac{U}{U^*} \right\} \cdot$$

$$\frac{dN_2}{d\xi} = 0 \quad (0.12)$$

$$\epsilon (1 + \epsilon) \quad 1 - \frac{3}{5} \frac{1 + \alpha\beta}{1 + \alpha\beta^2} \frac{dN_1}{d\xi} =$$

$$\left\{ -A_2 (1 - \epsilon) + \alpha X_{12} (-4A_1 \frac{\beta(1 + \epsilon\beta)}{(1 + \beta)^2} + \right.$$

$$\frac{4}{5} A_1 \frac{\beta(1 + \epsilon)}{(1 + \beta)^2} \frac{(1 + \alpha\beta)}{(1 + \alpha)} - 2A_2 \left( \frac{\beta}{1 + \beta} \right)^2 (1 - \epsilon) \left. \right\} N_1$$

$$+ X_{12} \left\{ 4A_1 \frac{\beta(\epsilon + \beta)}{(1 + \beta)^2} - \frac{4}{5} \frac{\beta(1 + \epsilon)}{(1 + \beta)^2} \frac{1 + \alpha\beta}{1 + \alpha} - \right.$$

$$2A_2 \left( \frac{\beta}{1 + \beta} \right)^2 (1 - \epsilon) \left. \right\} N_2 + A_2 (1 - \epsilon) N_1^2 +$$

$$X_{12} \left\{ 4A_1 \frac{\beta(1-\beta)}{(1+\beta)^2} (1-\epsilon) + 4A_2 \left( \frac{\beta}{1+\beta} \right)^2 (1-\epsilon) \right\}.$$

(0.13)

•  $N_1 N_2$ 

$$\begin{aligned} \epsilon (1+\epsilon) \left\{ 1 - \frac{3}{5} \frac{1+\infty\beta}{\beta(1+\infty)} \right\} \frac{dN_2}{d\xi} = \\ \infty X_{12} \left\{ 4A_1 \frac{1+\beta}{(1+\beta)^2} - \frac{4}{5} A_1 \frac{(1+\epsilon)}{(1+\beta)^2} \frac{1+\infty\beta}{1+\infty} - \right. \\ \left. 2A_2 \frac{1-\epsilon}{(1+\beta)^2} \right\} N_1 + \\ \left\{ -\infty X_{22} A_2 (1-\epsilon) + X_{12} (-4A_1 \frac{\beta+\epsilon}{(1+\beta)^2} + \frac{4}{5} A_1 \frac{1+\epsilon}{(1+\beta)^2} \right. \\ \left. \frac{1+\infty\beta}{1+\infty} - 2A_2 \frac{1-\epsilon}{(1+\beta)^2} \right\} N_2 + X_{22} A_2 (1-\epsilon) N_2^2 + \\ X_{12} \left\{ \frac{-4A_1 (1-\beta)(1-\epsilon)}{(1+\beta)^2} + 4A_2 \frac{1-\epsilon}{(1+\beta)^2} \right\}. \end{aligned}$$

(0.14)

 $N_1 N_2$ 

$$\text{Where } \epsilon = \frac{1}{4} \left( 1 + \frac{3}{M^2} \right)$$

$$\text{and } M^2 = U^2 / \left( \frac{2}{3} c_p T \right)$$

and the boundary conditions are

$$\lim_{x \rightarrow \infty} N_1 = 1, \quad N_1^+ = 0$$

$$N_2 = 0, \quad N_2^+ = 0 \quad (0.15)$$

Tanzenbaum and Scott (1966) pointed out that the formulation of the above mentioned problem was inconsistent in as much as the constancy of  $U^*$  and  $T^*$  implied that component gases would not separate. Tanzenbaum and Scott concluded that the mixture problem could not be solved using bi-modal description.

In view of the above we shall discuss in chapter I the formulation of the following problem for the mixture:

- I. Multimodal distribution function
- II. Bimodal distribution function of the components with suitable modification.

The discussion of the equations of problem II and their solution comprise chapter II which is the main body of the thesis.

As has been said earlier the shock wave structure

in the Mott-Smith theory depends upon the particular extra moment chosen and this arbitrariness is one of the shortcomings of this method. The study of this arbitrariness was initiated by Mott-Smith himself and he presented two solutions corresponding to  $c_x^2$  and  $c_x^3$  moments. Rosen (1954) attempted to remove this arbitrariness by means of a restricted variational principle. Gustafson (1960) showed that the restricted variational equation used by Rosen was a special case of a transfer equation and Oberai (1967) pointed out the non-uniqueness of Rosen's method. Later Narasimha (1966) proved that to every restricted variational principle there corresponds a transfer equation. However, one way to remove the arbitrariness is to find out that bimodal distribution which has a minimum deviation, in the least square sense, from the exact solution which, of course, is unknown (Oberai (1967)). However, this procedure necessitates the calculation of the collision integral itself, instead of its moments. Oberai presented solution only for the special case of  $M \rightarrow \infty$  and rigid sphere gas because in this case the upstream Maxwellian becomes a delta function and integration in the velocity space can be performed directly. Later, Narasimha and Deshpande (1969) obtained shock wave structure for the case of arbitrary Mach number using

this criterion by expressing the collision integral in closed form and evaluating the integrals needed in the formulation of the governing equations numerically.

The criterion to remove the arbitrariness can be applied to the mixture problem. In chapter III we shall discuss the formulation of the mixture problem for the case of arbitrary Mach number and present the solution for the special case of  $M \rightarrow \infty$  and rigid sphere molecules.

\*\*\*\*\*

## CHAPTER I



In this chapter we shall formulate the problem for a binary gas mixture retaining the essential features of the Mott-Smith ansatz. A simple minded approach will be to write the distribution functions for different gases as follows:

$$f_i = N_i^- (x) (2\pi R_i T)^{-\frac{3}{2}} \exp \left\{ -\frac{(\underline{c} - U_i)^2}{2 R_i T} \right\} +$$

$$N_i^+ (x) (2\pi R_i T^*)^{-\frac{3}{2}} \exp \left\{ -\frac{(\underline{c} - U_i^*)^2}{2 R_i T^*} \right\}$$

for  $i = 1, 2$  (1.1 a)  
b

$U$  and  $T$  are upstream velocity and temperature.  $U^*$  and  $T^*$ , though unknowns are postulated to be constants. So that in all, there are six unknowns:  $N_1^-$ ,  $N_1^+$ ,  $N_2^-$ ,  $N_2^+$ ,  $U^*$  and  $T^*$  and the boundary conditions are the following :

$$x \rightarrow -\infty, \quad N_1^- = 1, \quad N_2^- = \alpha$$

$$N_1^+ = N_2^+ = 0 \quad (1.2a)$$

$$x \rightarrow +\infty \quad N_1^- = N_2^- = 0 \quad (1.2b)$$

Boundary conditions (1.2b) imply that  $U^*$  and  $T^*$  are the downstream values of velocity and temperature. This was done by Oberai in 1965.

The conservation equations are the following:

$$\frac{d}{dx} \left[ U N_1^- + U^* N_1^+ \right] = 0 \quad (1.3)$$

$$\frac{d}{dx} \left[ U N_2^- + U^* N_2^+ \right] = 0 \quad (1.4)$$

$$\frac{d}{dx} \left\{ \sum_{i=1}^2 m_i \left[ N_i^- (U^2 + R_i T) + N_i^+ (U^{*2} + R_i T^*) \right] \right\} = 0 \quad (1.5)$$

$$\frac{d}{dx} \left\{ \sum_{i=1}^2 m_i \left[ N_i^- U (U^2 + 5R_i T) + N_i^+ U^* (U^{*2} + 5R_i T^*) \right] \right\} = 0 \quad (1.6)$$

Integrating the above equations (1.3) - (1.6) and evaluating the constants of integration from the upstream conditions, we obtain

$$N_1^- = 1 - \frac{U^*}{U} N_1^+ \quad (1.7)$$

$$N_2^- = \infty - \frac{U^*}{U} N_2^+ \quad (1.8)$$

$$\sum_{i=1}^2 m_i N_i^+ \left[ U (U^{*2} + R_i T^*) - U^* (U^2 + R_i T) \right] = 0 \quad (1.9)$$

$$\sum_{i=1}^2 m_i N_i^+ \left[ (U^{*2} + 5R_i T^*) - (U^2 + 5R_i T) \right] = 0 \quad (1.10)$$

Equations (1.9) and (1.10) can be solved for  $U^*$  and  $T^*$ . Ignoring the trivial solution

$$U = U^* \quad \text{and}$$

$$T = T^*,$$

we get

$$\frac{U^*}{U} = \frac{1}{4} \left( 1 + \frac{5 R_1 T}{U^2} \frac{N_1^+ + N_2^+}{N_1^+ + \beta N_2^+} \right) \quad (1.11)$$

$$\text{and } \frac{T^*}{T} = 1 + \frac{U^2}{5 R_1 T} \left[ 1 - \left( \frac{U^*}{U} \right)^2 \right] \left[ \frac{N_1^+ + \beta N_2^+}{N_1^+ + N_2^+} \right] \quad (1.12)$$

Where  $\beta = \frac{R_1}{R_2} = \frac{m_2}{m_1}$  ,

$m_1$  is the molecular mass of the first gas and  $m_2$  is the molecular mass of the second gas.

As  $U^*$  and  $T^*$  have already been postulated to be constants equations (1.11) and (1.12) imply that the expression

$$\frac{N_1^+ + N_2^+}{N_1^+ + \beta N_2^+}$$

does not depend on  $x$  throughout the shock wave - and hence is a constant. Equations (1.7) and (1.8) imply the relation

$$\frac{N_1^+}{N_2^+} = \frac{1 - N_1^-}{\infty - N_2^-}$$

and the boundary condition (1.2b) implies that

$$\text{Lt}_{x \rightarrow \infty} \frac{N_1^+}{N_2^+} \quad (\text{def}) \quad = \frac{N_1^*}{N_2^*} = \frac{1}{\infty}$$

The constant value of the expression

$$\frac{N_1^+ + N_2^+}{N_1^+ + \beta N_2^+}$$

must equal to

$$\frac{N_1^* + N_2^*}{N_1^* + \beta N_2^*} = \frac{1 + \infty}{1 + \infty/\beta}$$

$$\text{or} \quad \frac{N_2^+}{N_1^+} = \infty \quad (1.13)$$

(1-13) along with (1.7) and (1.8) implies

$$\frac{N_2^-}{N_1^-} = \infty$$

throughout the shock wave so that the ratio of the gas densities viz.  $\frac{N_2^- + N_2^+}{N_1^- + N_1^+}$  equal  $\infty$  for all points of the shockwave. This was pointed out by *Tanenbaum* and *Scott*(1966 ) who concluded that the mixture problem cannot be solved via a bimodal ansatz.

We shall examine whether the above shortcoming can be overcome by assuming distribution function to be trimodal in character.

We assume

$$f_1 = M_{11} + M_{12} + M_{13} \quad \text{and} \quad (1.14)$$

$$f_2 = M_{21} + M_{22} + M_{23} \quad (1.15)$$

where  $M_{11} = M(N_1^-, U, T, R_1)$

$$M_{12} = M(N_1^+, U^*, T^*, R_1)$$

$$M_{13} = M(n_1, U^*, T^*, R_2)$$

$$M_{21} = M(N_2^-, U, T, R_2)$$

$$M_{22} = M(N_2^+, U^*, T^*, R_2)$$

$$M_{23} = M(n_2, U^*, T^*, R_1)$$

where  $M(N, U, T, R)$  denotes

$$N(x) (2\pi RT)^{-3/2} \exp \left\{ -\frac{(c - U_1)^2}{2RT} \right\}$$

The choice of  $M_{13}$  and  $M_{23}$  is dictated by the consideration of simplicity, i.e., the problem should remain tractable. There are 8 unknowns namely  $N_1^-$ ,  $N_1^+$ ,  $n_1$ ,  $n_2$ ,  $N_2^-$ ,  $N_2^+$ ,  $U^*$  and  $T^*$  and the boundary conditions are the following.

$$x \rightarrow -\infty, N_1^- = 1, N_2^- = \infty, N_1^+ = N_2^+ = n_1 = n_2 = 0$$

$$x \rightarrow +\infty, N_1^- = N_2^- = n_1 = n_2 = 0$$

The derivation of the conservation equations is a standard one (see for example Oberai (1965)) and only the final results are given below:

$$\frac{d}{dx} [N_1^- U + N_1^+ U^* + n_1 U^*] = 0 \quad (1.16)$$

$$\frac{d}{dx} [N_2^- U + N_2^+ U^* + n_2 U^*] = 0 \quad (1.17)$$

$$\begin{aligned} \frac{d}{dx} \left\{ m_1 \left[ N_1^- (U^2 + R_1 T) + N_1^+ (U^{*2} + R_1 T^*) + n_1 (U^{*2} + R_2 T^*) \right] \right. \\ \left. + m_2 \left[ N_2^- (U^2 + R_2 T) + N_2^+ (U^{*2} + R_2 T^*) + n_2 (U^{*2} + R_1 T^*) \right] \right\} \\ = 0 \end{aligned} \quad (1.18)$$

$$\begin{aligned} \frac{d}{dx} \left\{ m_1 \left[ N_1^- U (U^2 + 5R_1 T) + N_1^+ U^* (U^* + 5R_1 T^*) + n_1 U^* \right. \right. \\ \left. \left. (U^{*2} + 5R_2 T^*) \right] + \right. \\ \left. m_2 \left[ N_2^- U (U^2 + 5R_2 T) + N_2^+ U^* (U^{*2} + 5R_2 T^*) + n_2 U^* \right. \right. \\ \left. \left. (U^{*2} + 5R_1 T^*) \right] \right\} = 0 \end{aligned} \quad (1.19)$$

If, after integrating the system of equations (1.16) to (1.19) and evaluating the constants of integration from the upstream conditions, one expresses  $\frac{U^*}{U}$  and  $\frac{T^*}{T}$  in terms of  $N_1^-$  and  $N_2^-$  etc. one gets

$$\frac{U^*}{U} = \frac{1}{4} + \frac{5}{4} \frac{R_1 T}{U^2} \frac{1 + \alpha - N_1^- - N_2^-}{1 + \alpha \beta - N_1^- - N_2^- \beta} \quad (1.20)$$

$$\text{and } \frac{T^*}{T} = \frac{(1 - N_1^-) (1 + \alpha + (1 - \epsilon^2) (1 + \alpha \beta) \frac{U^2}{5 R_1 T})}{\left[ \epsilon \frac{\beta - 1}{\beta} (N_1^+ - \beta N_2^+) + \frac{1}{\beta} (1 - N_1^-) (1 + \alpha \beta^2) \right]} \quad (1.21)$$

$$\text{Where } \epsilon = \frac{1}{4} + \frac{5}{4} \frac{R_1 T}{U^2} \frac{1 + \alpha}{1 + \alpha \beta}$$

$$\text{and } \beta = m_2/m_1$$

Equations (1.20) and (1.21) explicitly show that for the formulation to be consistent, two extra conditions are needed, namely,

$$N_1^- \alpha = N_2^- \quad (1.22)$$

$$\text{and } N_2^+ = \frac{N_1^+}{\beta} - \frac{(1 - N_1^-) (1 - \alpha \beta)}{\epsilon \beta} \quad (1.23)$$

These are artificial restrictions (predetermining separation) and resemble the one pointed out by Tannenbaum in the bimodal description.

Addition of one more Maxwellian in the distribution function makes the problem formidably complicated, without helping remove the shortcoming. We conclude that multimodal description does not lead to a physically acceptable solution of the mixture problem.

The second way to attack the problem is to modify the bimodal description in such a way that the above mentioned inconsistency does not arise. This was done by Oberai in 1966. He postulated the distribution function in the following form:

$$f_1 = N_1^-(x) (2\pi R_1 T)^{-\frac{3}{2}} \exp \left( -\frac{(\underline{c} - \underline{U}_1)^2}{2R_1 T} \right) + N_1^+(x) \left[ 2\pi R_1 T^+(x) \right]^{-\frac{3}{2}} \exp \left[ -\frac{(\underline{c} - \underline{U}^+(x)\underline{i})^2}{2R_1 T^+(x)} \right] \quad (1.24)$$

and

$$f_2 = N_2^-(x) (2\pi R_2 T)^{-\frac{3}{2}} \exp \left[ -\frac{(\underline{c} - \underline{U}_1)^2}{2R_2 T} \right] + N_2^+(x) \left[ 2\pi R_2 T^+(x) \right]^{-\frac{3}{2}} \exp \left[ -\frac{(\underline{c} - \underline{U}^+(x)\underline{i})^2}{2R_2 T^+(x)} \right] \quad (1.25)$$

with the conditions

$$x \rightarrow -\infty \quad N_1^- = 1, \quad N_2^- = \infty, \quad N_1^+ = N_2^+ = 0 \quad (1.25a)$$

$$x \rightarrow +\infty \quad N_1^- = N_2^- = 0$$

The following are the conservation equations when the distribution function  $f$  is as given in the equation (1.24 - 1.25)

$$\frac{d}{dx} \left[ UN_1^- + U^+ N_1^+ \right] = 0 \quad (1.26)$$

$$\frac{d}{dx} \left[ UN_2^- + U^+ N_2^+ \right] = 0 \quad (1.27)$$

$$\frac{d}{dx} \left\{ \sum_{i=1}^2 m_i \left[ N_i^- (U^2 + R_i T) + N_i^+ (U^{+2} + R_i T^+) \right] \right\} = 0 \quad (1.28)$$

$$\frac{d}{dx} \left\{ \sum_{i=1}^2 m_i \left[ N_i^- U (U^2 + 5R_i T) + N_i^+ U^+ (U^{+2} + 5R_i T^+) \right] \right\} = 0 \quad (1.29)$$

Integrating equations 1.26 - 1.29 and evaluating the constants of integration from the upstream conditions, we obtain

$$N_1^- = 1 - \frac{U^+}{U} N_1^+ \quad (1.30)$$

$$N_2^- = \infty - \frac{U^+}{U} N_2^+ \quad (1.31)$$

$$\sum_{i=1}^2 m_i N_i^+ \left[ U (U^{+2} + R_i T^+) - U^+ (U^2 + R_i T) \right] = 0 \quad (1.32)$$

$$\sum_{i=1}^2 m_i N_i^+ \left[ (U^{+2} + 5R_i T^+) - (U^2 + 5R_i T) \right] = 0 \quad (1.33)$$

Equations (1.32) and (1.33) can be solved for  $U^+$  and  $T^+$ . Ignoring the trivial solution  $U = U^+$  and  $T = T^+$ , we get

$$\frac{U^+}{U} = \frac{1}{4} \left[ 1 + \frac{5R_1 T}{U^2} \frac{N_1^+ + N_2^+}{N_1^+ + \beta N_2^+} \right] \quad (1.34)$$

$$\frac{T^+}{T} = 1 + \frac{U^2}{5R_1 T} \left[ 1 - \left( \frac{U^+}{U} \right)^2 \right] \frac{N_1^+ + \beta N_2^+}{N_1^+ + N_2^+} \quad (1.35)$$



where  $\beta = \frac{m_2}{m_1}$ , the ratio of the molecular masses

Using the four conservation equations, four unknowns  $N_1^-$ ,  $N_2^-$ ,  $U^+$ ,  $T^+$  have been expressed in terms of  $N_1^+$  and  $N_2^+$ . The functions  $N_1^+$  and  $N_2^+$  are to be determined from additional transfer equations. No inconsistency arises because  $U^+$  and  $T^+$  are already functions of  $x$  thereby allowing for separation of the species.

Limiting value of any function of interest at downstream infinity will be denoted by asterisk e.g.  $N_i^*$  denotes  $N_i(x)$  when  $x$  approaches  $+\infty$

Taking the limit of the equations  $\begin{matrix} (1.34) \\ (1.30) \end{matrix}$  and  $\begin{matrix} (1.35) \\ (1.31) \end{matrix}$  as  $x \rightarrow \infty$  and making use of  $\zeta$  and  $\zeta$ , we have

$$\frac{(U^+)^*}{U} = \frac{1}{4} \left( 1 + \frac{1 + \infty}{1 + 2\beta} \frac{5R_1 T}{U^2} \right) = \zeta \text{ (say)} \quad (1.36)$$

$$\frac{(T^+)^*}{T} = 1 + \frac{1 - \zeta^2}{4\zeta - 1} \quad (1.37)$$

$$N_1^* = \frac{1}{\zeta} \quad (1.38)$$

$$N_2^* = \frac{\infty}{\zeta} \quad (1.39)$$

Relations 1.36 to 1.39 may be recognised as the Rankine Hugoniot relations if we observe that the expression for  $C_p$ , the specific heat at constant pressure, of the mixture, evaluated upstream is

$$C_p = \frac{5R_1}{2} \frac{1 + \infty}{1 + \infty\beta}$$

so that the upstream Mach number  $M$  which is defined as

$$M^2 = U^2 \left( \frac{2}{3} C_p T \right)^{-1}$$

is related to  $\epsilon$  as follows:

$$\epsilon = \frac{1}{4} \left( 1 + \frac{3}{M^2} \right)$$

Oberai took  $c_x^2$  moment for Maxwell molecules to determine the shock structure and presented the solution for small values of the concentration ratio. The transfer equations with  $c_x^2$  moment are the following.

$$\begin{aligned} \frac{d}{d\xi} \left\{ \frac{U^+}{U} N_1^+ \left[ 3R_1 (T^* - T) - (U^2 - U^{+2}) \right] \right\} = \\ x_{12} \left\{ \frac{4A_1\beta}{1+\beta} \left[ \left( 1 - \frac{U^+}{U} N_1^+ \right) N_2^+ (UU^+ - U^{+2}) \right. \right. \\ \left. \left. + \left( \infty - \frac{U^+}{U} N_2^+ \right) N_1^+ (UU^+ - U^{+2}) + (N_2^+ - \infty N_1^+) \frac{R_1(T^+ - T)}{1+\beta} \right] \right. \\ \left. + (4A_1 - 2A_2) \left( \frac{\beta}{1+\beta} \right)^2 (N_2^+ + \infty N_1^+ - \frac{2U^+}{U} N_1^+ N_2^+) \right. \\ \left. (U - U^+)^2 \right\} - A_2 \left( 1 - \frac{U^+}{U} N_1^+ \right) N_1^+ (U - U^+)^2 \quad (1.40) \end{aligned}$$

$$\begin{aligned} \frac{d}{d\xi} \left\{ \frac{U^+}{U} N_2^+ \left[ 3R_2 (T^+ - T) - (U^2 - U^{+2}) \right] \right\} = \\ x_{12} \left\{ \frac{4A_1}{1+\beta} \left[ \left( \infty - \frac{U^+}{U} N_2^+ \right) N_1^+ (UU^+ - U^2) + \left( 1 - \frac{U^+}{U} N_1^+ \right) \right. \right. \\ \left. \left. N_2^+ (UU^+ - U^{+2}) + (\infty N_1^+ - N_2^+) \frac{R_1(T^+ - T)}{1+\beta} \right] \right. \\ \left. + \frac{4A_1 - 2A_2}{(1+\beta)^2} (N_2^+ + \infty N_1^+ - 2 \frac{U^+}{U} N_1^+ N_2^+) (U - U^+)^2 \right\} \end{aligned}$$

$$- x_{22} A_2 \left( \infty - \frac{U^+}{U} N_2^+ \right) N_2^+ (U - U^+)^2 \quad (1.41)$$

$$\text{Where } \xi = x/L \text{ with } L = \left( \frac{U}{\pi N_0} \right) \left( \frac{m_1}{2K_{11}} \right)^{1/2}$$

$$\text{and } x_{12} = \left( \frac{m_1 + m_2}{2m_2} \quad \frac{K_{12}}{K_{11}} \right)^{1/2}$$

$$x_{22} = \sqrt{\frac{m_1}{m_2} \quad \frac{K_{22}}{K_{11}}}$$

and  $A_1, A_2$  are certain integrals for Maxwell molecules discussed in the appendix.

We also give here below the  $C_x^3$  moment transfer equations for Maxwell molecules:

$$\begin{aligned} \frac{d}{d\xi} \left[ N_1^- (U^4 + 6U^2 R_1 T + 3R_1^2 T^2) + N_1^+ (U^{+4} + 6U^{+2} R_1 T^+ + 3R_1^2 T^{+2}) \right] = \\ \left\{ Z_3 \left[ UU^+ (U^2 + R_1 T) - U^2 (U^{+2} + 3R_1 T) \right] + \right. \\ Z_4 \left[ U^2 (U^{+2} + R_1 T^+) + U^2 (U^2 + 3R_1 T) - 2UU^+ (U^2 + R_1 T) \right] + \\ Z_5 \left[ U^2 (2R_1 T + 2R_1 T^+) \right] + Z_3 \left[ U^2 (U^{+2} + R_1 T^+) - \right. \\ \left. UU^+ (U^{+2} + 3R_1 T^+) \right] \\ \left. + Z_4 \left[ UU^+ (U^2 + R_1 T) + UU^+ (U^{+2} + 3R_1 T^+) - 2U^2 (U^{+2} + R_1 T^+) \right] \right. \\ \left. + Z_5 \left[ UU^+ (2R_1 T + 2R_1 T^+) \right] \right\} N_1^- N_1^+ \\ + x_{12} \left\{ (AZ_1 \left[ UU^+ (U^{+2} + 3R_2 T^+) - 3U^2 (U^{+2} + R_2 T^+) + \right. \right. \end{aligned}$$

$$\begin{aligned}
& 3UU^+ (U^2 + R_1 T) - U^2 (U^2 + 3R_1 T) \Big] + AZ2 \Big[ (UU^+ - U^2) \\
& (2R_2 T^+ + 2R_1 T) \Big] + AZ3 \Big[ UU^+ (U^2 + R_1 T) - U^2 (U^{+2} + 3R_1 T) \Big] \\
& + AZ4 \Big[ U^2 (U^{+2} + R_2 T^+) + U^2 (U^2 + 3R_1 T) - 2U^+ U (U^2 + R_1 T) \Big] \\
& + AZ5 \Big[ U^2 (2R_2 T^+ + 2R_1 T) \Big] \Big\} N_1^- N_2^+ + \\
& x_{12} \Big\{ AZ1 \Big[ U^2 (U^2 + 3R_2 T) - 3U^+ U (U^2 + R_2 T) + 3U^2 \\
& (U^{+2} + R_1 T^+) - U^+ U (U^{+2} + 3R_1 T^+) \Big] + AZ2 \Big[ (2R_2 T + 2R_1 T^+) \\
& (U^2 - U^+ U) \Big] + \\
& AZ3 \Big[ U^2 (U^{+2} + R_1 T^+) - U^+ U (U^{+2} + 3R_1 T^+) \Big] + \\
& AZ4 \Big[ U^+ U (U^2 + R_2 T) + UU^+ (U^{+2} + 3R_1 T^+) - 2U^2 (U^{+2} + R_1 T^+) \Big] \\
& + AZ5 \Big[ UU^+ (2R_2 T + 2R_1 T^+) \Big] \Big\} N_1^+ (x) N_2^- (x) \quad (1.42)
\end{aligned}$$

and

$$\begin{aligned}
& \frac{d}{d\xi} \Big[ N_2^- (U^4 + 6U^2 R_2 T + 3R_2^2 T^2) + N_2^+ (U^{+4} + 6U^{+2} R_2 T^+ \\
& + 3R_2^2 T^{+2}) \Big] = \\
& x_{12} \Big\{ BZ1 \Big[ UU^+ (U^{+2} + 3R_2 T^+) - 3U^2 (U^{+2} + R_2 T^+) + 3UU^+ \\
& (U^2 + R_1 T) - U^2 (U^2 + 3R_1 T) \Big] + BZ2 \Big[ (UU^+ - U^2) \\
& (2R_2 T^+ + 2R_1 T) \Big] + BZ3 \Big[ (UU^+ (U^{+2} + 3R_2 T^+) - U^2 (U^{+2} + R_2 T^+)) \Big] \\
& + BZ4 \Big[ UU^+ (U^{+2} + 3R_2 T^+) + UU^+ (U^2 + R_1 T) - 2U^2 (U^{+2} + R_2 T^+) \Big] +
\end{aligned}$$

$$\begin{aligned}
& \text{BZ5} \left[ (UU^+ (2R_2T^+ + 2R_1T)) \right] \left\{ N_1^- (x) N_2^+ (x) + \right. \\
& x_{12} \left\{ \text{BZ1} \left[ U^2 (U^2 + 3R_2T) - 3UU^+ (U^2 + R_2T) + 3U^2 \right. \right. \\
& (U^{+2} + R_1T^+) - UU^+ (U^{+2} + 3R_1T^+) \left. \right] + \text{BZ2} \left[ (U^2 - UU^+) \right. \\
& (2R_2T + 2R_1T^+) \left. \right] + \text{BZ3} \left[ U^2 (U^2 + 3R_2T) - UU^+ (U^2 + R_2T) \right] \\
& + \text{BZ4} \left[ U^2 (U^2 + 3R_2T) + U^2 (U^{+2} + R_1T^+) - 2UU^+ (U^2 + R_2T) \right] \\
& + \text{BZ5} \left[ U^2 (2R_2T + 2R_1T^+) \right] \left. \right\} N_2^- (x) N_1^+ (x) + \\
& x_{22} \left\{ \text{CZ3} \left[ U^2 (U^2 + 3R_2T) - UU^+ (U^2 + R_2T) \right] + \right. \\
& \text{CZ4} \left[ U^2 (U^2 + 3R_2T) + U^2 (U^{+2} + R_2T^+) - 2UU^+ (U^2 + R_2T) \right] \\
& + \text{CZ5} \left[ U^2 (2R_2T + 2R_2T^+) \right] \left. \right\} N_2^- N_2^+ + \\
& x_{22} \left\{ \text{CZ3} \left[ U^+U (U^{+2} + 3R_2T^+) - U^2 (U^{+2} + R_2T^+) \right] + \right. \\
& \text{CZ4} \left[ U^+U (U^{+2} + 3R_2T^+) + U^+U (U^2 + R_2T) - 2UU^+ \right. \\
& (U^{+2} + R_2T^+) \left. \right] + \text{CZ5} \left[ U^+U (2R_2T^+ + 2R_2T) \right] \left. \right\} N_2^- N_2^+ \\
& (1.43)
\end{aligned}$$

where

$$\text{BZ1} = - \frac{2}{(1 + \beta)^3} (3A_1 - 3A_2 + A_3)$$

$$BZ2 = - \frac{3}{(1 + \beta)^3} (A_1 + A_2 - A_3)$$

$$BZ3 = -6A_1 / (1 + \beta)$$

$$BZ4 = 6 (2A_1 - A_2) / (1 + \beta)^2$$

$$BZ5 = 3A_2 / (1 + \beta)^2$$

$$CZ1 = -\frac{1}{4} (3A_1 - 3A_2 + A_3)$$

$$CZ2 = -\frac{3}{8} (A_1 + A_2 - A_3)$$

$$CZ3 = -3A_1$$

$$CZ4 = \frac{3}{2} (2A_1 - A_2)$$

$$CZ5 = \frac{3}{4} A_2$$

$$Z3 = 3A_1$$

$$Z4 = \frac{3}{2} (2A_1 - A_2)$$

$$Z5 = \frac{3}{4} A_2$$

$$AZ1 = 2(3A_1 - 2A_2 + A_3) \left[ \frac{\beta}{1+\beta} \right]^3$$

$$AZ2 = 3(A_1 + A_2 - A_3) \left[ \frac{\beta}{1+\beta} \right]^3$$

$$AZ3 = \frac{6\beta}{1+\beta} A_1$$

$$AZ4 = 6(2A_1 - A_2) \left[ \frac{\beta}{1+\beta} \right]^2$$

$$AZ5 = 3A_2 \left[ \frac{\beta}{1+\beta} \right]$$

and the  $c_x^2$ -moment transfer equations for rigid sphere molecular model.

$$\frac{d}{d\xi} \left\{ U^+ N_1^+ \left[ 3R_1 (T^+ - T) - (U^2 - U^{+2}) \right] \right\} =$$

$$- \frac{1}{3} \sqrt{\pi} \sigma_1^2 N_1^- N_1^+ \theta(s_1) \left[ 2R_1 (T + T^+) \right]^{3/2}$$

$$- N_1^- N_2^+ \sqrt{\pi} M_2^2 \sigma_{12}^2 \phi(s_{ud_1}, \omega_1, \eta_1) \left[ 2R_1 T + 2R_2 T^+ \right]$$

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$$-N_1^+ N_2^- \sqrt{\Lambda} M_2^2 \sigma_{12}^2 \phi(s_{ud_2}, \omega_2, \eta_2) \left[ 2R_1 T^+ + 2R_2 T \right]^{3/2} \quad (1.44)$$

and

$$\begin{aligned} \frac{d}{d\xi} \left\{ U^+ N_2^+ \left[ 3R_2 (T^+ - T) - (U_2^2 - U^{+2}) \right] \right\} = \\ - \frac{1}{3} \sqrt{\Lambda} \sigma_2^2 N_2^- N_2^+ \theta(s_2) (2R_2 T + 2R_2 T^+)^{3/2} \\ N_1^+ N_2^- \sqrt{\Lambda} M_1^2 \sigma_{12}^2 \phi(s_{ud_2}, \omega_3, \eta_3) \left[ 2R_1 T^+ + 2R_2 T \right]^{3/2} \\ - N_1^- N_2^+ \sqrt{\Lambda} M_1^2 \sigma_{12}^2 \phi(s_{ud_1}, \omega_4, \eta_4) \left[ 2R_1 T + 2R_2 T^+ \right]^{3/2} \end{aligned} \quad (1.45)$$

where

$$s_1 = (U - U^+) / \left[ 2R_1 (T + T^+) \right]^{1/2}$$

$$s_2 = (U - U^+) / \left[ 2R_2 (T + T^+) \right]^{1/2}$$

$$\theta(s) = (s^2 + 1 - \frac{3}{4s^2}) \exp(-s^2)$$

$$+ (2s^3 + 3s - \frac{3}{2s} + \frac{3}{4s^3}) \frac{1}{2} \operatorname{erf}(s) \sqrt{\Lambda}$$

$$M_1 = m_1 / (m_1 + m_2)$$

$$M_2 = m_2 / (m_1 + m_2)$$

$$\sigma_{12} = (\sigma_1 + \sigma_2) / 2$$

$$\omega_1 = \frac{T}{m_1 M_2 \left( \frac{T}{m_1} + \frac{T^+}{m_2} \right)}$$

$$\omega_2 = \frac{T^+}{m_1 M_2 \left( \frac{T^+}{m_1} + \frac{T}{m_2} \right)}$$

$$\omega_3 = \frac{T}{m_2 M_1 (T^+/m_1 + T/m_2)}$$

$$\omega_4 = \frac{T^*}{m_2 M_1 (T/m_1 + T^+/m_2)}$$

$$\eta_1 = \frac{2U}{M_2 (U - U^+)}$$

$$\eta_2 = \frac{2U^+}{M_2 (U - U^+)}$$

$$\eta_3 = \frac{2U}{M_1 (U - U^+)}$$

$$\eta_4 = \frac{2U^+}{M_1 (U - U^+)}$$

$$s_{ud_1} = (U - U^+)/\sqrt{(2R_1 T + 2R_2 T^+)}$$

$$s_{ud_2} = (U - U^+)/\sqrt{(2R_2 T + 2R_1 T^+)}$$

$$\begin{aligned} \phi(s, \omega, \eta) = & \left[ \left( \eta - \frac{4}{3} \right) s^2 + \left( 2\omega + \frac{1}{2} \right) \eta - \frac{7}{3} \right] \\ & + \left( \frac{1}{2} - \omega \right) s^{-2} \left] e^{-s^2} + \left[ \left( \omega - \frac{1}{2} \right) \frac{1}{s^3} - \frac{\eta}{2s} + (4\omega - 6 + 2\eta) s \right. \right. \\ & \left. \left. + 2 \left( \eta - \frac{4}{3} \right) s^3 \right] \frac{1}{2} \sqrt{\pi} \operatorname{erf}(s) \right. \end{aligned}$$

Detailed study of the problem for various values of concentration ratio, mass ratio and Mach Number is not reported in the literature. The main objective of the thesis is to discuss the nature of system 1.40, 1.41, 1.42, 1.43, 1.44, 1.45 and 1.25 and to present their



solutions for various sets of the values of  $(\alpha, \beta, M)$   
to bring out -

- i) The individual effect of these parameters
  - ii) A consistent trend, if any, in the  $c_x^2$  and  $c_x^3$   
moment solutions and
  - iii) The effect of molecular model on the shock  
structure.
-

## CHAPTER II

In the present investigation, the shock structure is determined provided the molecular model and the two additional velocity moments of the Boltzmann equations are prescribed.

The conservation of mass, momentum and energy yields the following governing equations:

$$\frac{d}{d\xi} \left[ N_1^- + \frac{U^+}{U} N_1^+ \right] = 0 \quad (2.1)$$

$$\frac{d}{d\xi} \left[ N_2^- + \frac{U^+}{U} N_2^+ \right] = 0 \quad (2.2)$$

$$\frac{d}{d\xi} \left\{ \sum_{i=1}^2 m_i \left[ N_i^- \left( 1 + \frac{R_i T}{U^2} \right) + N_i^+ \left( \left( \frac{U^+}{U} \right)^2 + \frac{R_i T}{U^2} \frac{T^+}{T} \right) \right] \right\} = 0 \quad (2.3)$$

$$\frac{d}{d\xi} \left\{ \sum_{i=1}^2 m_i \left[ N_i^- \left( 1 + \frac{5R_i T}{U^2} \right) + N_i^+ \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{5R_i T}{U^2} \frac{T^+}{T} \right\} \right] \right\} = 0 \quad (2.4)$$

leading to the following expression for  $N_1^-$ ,  $N_2^-$ ,

$$\frac{U^+}{U} \quad \text{and} \quad \frac{T^+}{T}$$

$$N_1^- = 1 - \frac{U^+}{U} N_1^+ \quad (2.5)$$

$$N_2^- = \infty - \frac{U^+}{U} N_2^+ \quad (2.6)$$

$$\frac{U^+}{U} \approx \frac{1}{4} \left( 1 + \frac{5R_1 T}{U^2} \frac{N_1^+ N_2^+}{N_1^+ + \beta N_2^+} \right) \quad (2.7)$$

$$\frac{T^+}{T} = 1 + \frac{U^2}{5R_1 T} \left[ 1 - \left( \frac{U^+}{U} \right)^2 \right] \frac{N_1^+ + \beta N_2^+}{N_1^+ + N_2^+} \quad (2.8)$$

For the remaining unknowns  $N_1^+$  and  $N_2^+$  we have to use two extra moment (transfer) equations. As in these extra transfer equations, the corresponding moment of the collision integral will not vanish, the molecular model will also play a part. To verify if the choice of the transfer equation and of the molecular model have a consistent trend in the final results, we shall study three different cases:

Case 1.  $a_x^2$  - moment and Maxwell molecule

$$\begin{aligned} \frac{d}{d\xi} \left\{ \frac{U^+}{U} N_1^+ \left[ \frac{3R_1 T}{U^2} \left( \frac{T^+}{T} - 1 \right) - \left( 1 - \left( \frac{U^+}{U} \right)^2 \right) \right] \right\} = \\ x_{12} \left\{ \frac{4A_1 \beta}{1+\beta} \left[ \left( 1 - \frac{U^+}{U} N_1^+ \right) N_2^+ - \frac{U^+}{U} \left( 1 - \frac{U^+}{U} \right) + \right. \right. \\ \left. \left( \infty - \frac{U^+}{U} N_2^+ \right) N_1^+ - \frac{U^+}{U} \left( 1 - \frac{U^+}{U} \right) + \right. \\ \left. \left( N_2^+ - \infty N_1^+ \right) \frac{R_1 T}{U^2} \frac{1}{1+\beta} \left( \frac{T^+}{T} - 1 \right) \right] + \\ \left. \left( 4A_1 - 2A_2 \right) \left( \frac{\beta}{1+\beta} \right)^2 \left[ N_2^+ + \infty N_1^+ - 2 \frac{U^+}{U} N_1^+ N_2^+ \right] \left( 1 - \frac{U^+}{U} \right)^2 \right\} \\ - A_2 \left( 1 - \frac{U^+}{U} N_1^+ \right) N_1^+ \left( 1 - \frac{U^+}{U} \right)^2 \quad (2.9a) \end{aligned}$$

$$\begin{aligned}
& \frac{d}{d\xi} \left\{ \frac{U^+}{U} N_2^+ \left[ \frac{3R_2 T}{U^2} \left( \frac{T^+}{T} - 1 \right) - \left( 1 - \left( \frac{U^+}{U} \right)^2 \right) \right] \right\} = \\
& x_{12} \left\{ \frac{4A_1}{1+\beta} \left[ \left( \alpha - \frac{U^+}{U} N_2^+ \right) N_1^+ \left( \frac{U^+}{U} - 1 \right) + \left( 1 - \frac{U^+}{U} N_1^+ \right) \right. \right. \\
& \left. \left. N_2^+ \frac{U^+}{U} \left( 1 - \frac{U^+}{U} \right) + \left( \alpha N_1^+ - N_2^+ \right) \frac{R_1 T}{U^2} \frac{1}{1+\beta} \left( \frac{T^+}{T} - 1 \right) \right] \right. \\
& \left. + \frac{(4A_1 - 2A_2)}{(1+\beta)^2} \left( N_2^+ + \alpha N_1^+ - 2 \frac{U^+}{U} N_1^+ N_2^+ \right) \left( 1 - \frac{U^+}{U} \right)^2 \right\} \\
& - x_{22} A_2 \left( \alpha - \frac{U^+}{U} N_2^+ \right) N_2^+ \left( 1 - \frac{U^+}{U} \right)^2 \quad (2.9b)
\end{aligned}$$

Case 2.  $\bar{o}_x^3$  - moment and Maxwell molecule :

$$\begin{aligned}
& \frac{d}{d\xi} \left[ N_1^+ \left( 1 + \frac{6R_1 T}{U^2} + \frac{3R_1^2 T^2}{U^4} \right) + N_1^+ \left\{ \left( \frac{U^+}{U} \right)^4 + 6 \left( \frac{U^+}{U} \right)^2 \right. \right. \\
& \left. \left. \frac{R_1 T}{U^2} \frac{T^+}{T} + \frac{3R_1^2 T^2}{U^4} \left( \frac{T^+}{T} \right)^2 \right\} \right] = \\
& \left\{ 3A_1 \left[ \frac{U^+}{U} \left( 1 + \frac{R_1 T}{U^2} \right) - \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_1 T}{U^2} \right\} \right] + \right. \\
& \left. \frac{3}{2} (2A_1 - A_2) \left[ \left( \frac{U^+}{U} \right)^2 + \frac{R_1 T}{U^2} \frac{T^+}{T} + 1 + \frac{3R_1 T}{U^2} - \right. \right. \\
& \left. \left. \frac{2U^+}{U} \left( 1 + \frac{R_1 T}{U^2} \right) \right] + \frac{3}{4} A_2 \left[ \frac{2R_1 T}{U^2} \left( 1 + \frac{T^+}{T} \right) \right] + 3A_1 \right. \\
& \left. \left[ \left( \frac{U^+}{U} \right)^2 + \frac{R_1 T}{U^2} \frac{T^+}{T} - \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_1 T}{U^2} \frac{T^+}{T} \right\} \right] + \frac{3}{2} \right. \\
& \left. (2A_1 - A_2) \left[ \frac{U^+}{U} \left( 1 + \frac{R_1 T}{U^2} \right) + \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_1 T}{U^2} \frac{T^+}{T} \right\} \right] \right\}
\end{aligned}$$

$$- 2 \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{R_1 T}{U^2} \frac{T^+}{T} \right\} \left] + \frac{3}{4} A_2 \left[ \frac{U^+}{U} \frac{2R_1 T}{U^2} \left( 1 + \frac{T^+}{T} \right) \right] \right\}$$

$$N_1^- N_1^+ + x_{12} \left\{ \left( \frac{\beta}{1+\beta} \right)^3 2 (3A_1 - 3A_2 + A_3) \right.$$

$$\left. \left[ \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_2 T}{U^2} \frac{T^+}{T} \right\} - 3 \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{R_2 T}{U^2} \frac{T^+}{T} \right\} + \right.$$

$$\left. 3 \frac{U^+}{U} \left( 1 + \frac{R_1 T}{U^2} \right) - \left( 1 + \frac{3R_1 T}{U^2} \right) \right] + \left( \frac{\beta}{1+\beta} \right)^3 \frac{3}{8}$$

$$(A_1 + A_2 - A_3) \left[ \left( \frac{U^+}{U} - 1 \right) \frac{2R_1 T}{U^2} \left( 1 + \frac{T^+}{T} \right) \right] *$$

$$\frac{\beta}{1+\beta} 6A_1 \left[ \frac{U^+}{U} \left( 1 + \frac{R_1 T}{U^2} \right) - \left( 1 + \frac{3R_1 T}{U^2} \right) \right] + \left( \frac{\beta}{1+\beta} \right)^2$$

$$6 (2A_1 - A_2) \left[ \left( \frac{U^+}{U} \right)^2 + \frac{R_2 T}{U^2} \frac{T^+}{T} + 1 + \frac{3R_1 T}{U^2} - 2 \frac{U^+}{U} \right. \\ \left. \left( 1 + \frac{R_1 T}{U^2} \right) \right] + \left( \frac{\beta}{1+\beta} \right)^2 3A_2 \left[ \frac{2R_1 T}{U^2} \left( 1 + \frac{T^+}{T} \right) \right] \left. \right\}$$

$$N_1^-(x) N_2^+(x) + x_{12} \left\{ \left( \frac{\beta}{1+\beta} \right)^3 2 (3A_1 - 3A_2 + A_3) \right.$$

$$\left[ \left( 1 + \frac{3R_1 T}{U^2} \right) - 3 \frac{U^+}{U} \left( 1 + \frac{R_2 T}{U^2} \right) + 3 \left\{ \left( \frac{U^+}{U} \right)^2 + \right.$$

$$\left. \frac{R_1 T}{U^2} \frac{T^+}{T} \right\} - \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_1 T}{U^2} \frac{T^+}{T} \right\} \left. \right] +$$

$$\left( \frac{\beta}{1+\beta} \right)^3 3(A_1 + A_2 - A_3) \left[ \frac{2R_2 T}{U^2} \left( 1 + \frac{T^+}{T} \right) \left( 1 - \frac{U^+}{U} \right) \right] +$$

$$\frac{\beta}{1+\beta} 6A_1 \left[ \left( \frac{U^+}{U} \right)^2 + \frac{R_1 T}{U^2} \frac{T^+}{T} - \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_1 T}{U^2} \frac{T^+}{T} \right\} \right] +$$

$$\begin{aligned}
& 6(2A_1 - A_2) \left( \frac{\beta}{1+\beta} \right)^2 \left[ \frac{U^+}{U} \left( 1 + \frac{R_2 T}{U^2} \right) + \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \right. \right. \\
& \left. \left. \frac{3R_1 T}{U^2} \frac{T^+}{T} \right\} - 2 \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{R_1 T}{U^2} \frac{T^+}{T} \right\} \right] + 3 \left( \frac{\beta}{1+\beta} \right)^2 A_2 \\
& \left[ \frac{2R_2 T}{U^2} \left( 1 + \beta \frac{T^+}{T} \right) \frac{U^+}{U} \right] N_1^+ N_2^- \quad (2.10a)
\end{aligned}$$

and

$$\begin{aligned}
& \frac{d}{d\xi} \left\{ N_2^- \left[ \left( 1 + \frac{6R_2 T}{U^2} \right) + \frac{3R_2^2 T^2}{U^4} \right] + N_2^+ \left[ \left( \frac{U^+}{U} \right)^4 + \right. \right. \\
& \left. \left. 6 \left( \frac{U^+}{U} \right)^2 \frac{R_2 T}{U^2} \frac{T^+}{T} + \frac{3R_2^2 T^2}{U^4} \left( \frac{T^+}{T} \right)^2 \right] \right\} = \\
& x_{12} \left\{ \frac{-2(3A_1 - 3A_2 + A_3)}{(1+\beta)^3} * \left[ \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \right. \right. \right. \\
& \left. \left. \frac{3R_2 T}{U^2} \frac{T^+}{T} \right\} - 3 \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{R_2 T}{U^2} \frac{T^+}{T} \right\} + 3 \frac{U^+}{U} \left( 1 + \frac{R_1 T}{U^2} \right) \right. \\
& \left. \left. - \left( 1 + \frac{3R_1 T}{U^2} \right) \right] - \frac{3(A_1 + A_2 - A_3)}{(1+\beta)^3} \left[ \frac{2R_1 T}{U^2} \left( 1 + \frac{T^+}{T} \right) \right. \right. \\
& \left. \left. \left( \frac{U^+}{U} - 1 \right) \right] - \frac{6A_1}{1+\beta} \left[ \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_2 T}{U^2} \frac{T^+}{T} \right\} - \right. \right. \\
& \left. \left. \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{R_2 T}{U^2} \frac{T^+}{T} \right\} \right] + \frac{6(2A_1 - A_2)}{(1+\beta)^2} * \right. \\
& \left[ \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_2 T}{U^2} \frac{T^+}{T} \right\} + \frac{U^+}{U} \left( 1 + \frac{R_1 T}{U^2} \right) - \right. \\
& \left. \left. 2 \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{R_2 T}{U^2} \frac{T^+}{T} \right\} \right] + \frac{3A_2}{(1+\beta)^2} \left[ \frac{2R_1 T}{U^2} \left( 1 + \frac{T^+}{T} \right) \frac{1}{\beta} \right) \right]
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{U^+}{U} \right] \left. N_1^- N_2^+ \right. + x_{22} \left[ - \frac{2(3A_1 - 3A_2 + A_3)}{(1 + \beta)^3} \right. \\
& \left. \left\{ \left( 1 + \frac{3R_{2T}}{U^2} \right) - 3 \frac{U^+}{U} \left( 1 + \frac{R_{2T}}{U^2} \right) + 3 \left[ \left( \frac{U^+}{U} \right)^2 + \right. \right. \right. \\
& \left. \left. \frac{R_{1T}}{U^2} \frac{T^+}{T} \right] - \frac{U^+}{U} \left[ \left( \frac{U^+}{U} \right)^2 + \frac{3R_{1T}}{U^2} \frac{T^+}{T} \right] \right\} - \frac{3(A_1 + A_2 - A_3)}{(1 + \beta)^3} \\
& \left\{ \frac{2R_{2T}}{U^2} \left( 1 + \beta \frac{T^+}{T} \right) \left( 1 - \frac{U^+}{U} \right) \right\} - \frac{6A_1}{(1 + \beta)} \left\{ \left( 1 + \frac{3R_{2T}}{U^2} \right) \right. \\
& \left. - \frac{U^+}{U} \left( 1 + \frac{R_{2T}}{U^2} \right) \right\} + \frac{6(2A_1 - A_2)}{(1 + \beta)^2} \left\{ \left( 1 + \frac{3R_{2T}}{U^2} \right) + \right. \\
& \left. \left[ \left( \frac{U^+}{U} \right)^2 + \frac{R_{1T}}{U^2} \frac{T^+}{T} \right] - 2 \frac{U^+}{U} \left( 1 + \frac{R_{2T}}{U^2} \right) \right\} + \\
& \frac{3A_2}{(1 + \beta)^2} \left\{ \frac{2R_{2T}}{U^2} \left( 1 + \beta \frac{T^+}{T} \right) \right\} \left. N_2^-(x) N_1^+(x) \right. + \\
& x_{22} \left\{ - 3A_1 \left[ \left( 1 + \frac{3R_{2T}}{U^2} \right) - \frac{U^+}{U} \left( 1 + \frac{R_{2T}}{U^2} \right) \right] + \right. \\
& \frac{3}{2} (2A_1 - A_2) \left[ \left( 1 + \frac{3R_{2T}}{U^2} \right) + \left( \frac{U^+}{U} \right)^2 + \frac{R_{2T}}{U^2} \frac{T^+}{T} - \right. \\
& \left. 2 \frac{U^+}{U} \left( 1 + \frac{R_{2T}}{U^2} \right) \right] + \frac{3}{4} A_2 \left[ \frac{2R_{2T}}{U^2} \left( 1 + \frac{T^+}{T} \right) \right] \left. N_2^-(x) N_2^+(x) \right. + \\
& x_{22} \left\{ - 3A_1 \left[ \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_{2T}}{U^2} \frac{T^+}{T} \right\} - \left\{ \left( \frac{U^+}{U} \right)^2 + \right. \right. \right. \\
& \left. \left. \frac{R_{2T}}{U^2} \frac{T^+}{T} \right\} \right] + \frac{3}{2} (2A_1 - A_2) \left[ \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{3R_{2T}}{U^2} \frac{T^+}{T} \right\} + \right.
\end{aligned}$$



$$\frac{U^+}{U} \left( 1 + \frac{R_2 T}{U^2} \right) - 2 \frac{U^+}{U} \left\{ \left( \frac{U^+}{U} \right)^2 + \frac{R_2 T}{U^2} \frac{T^+}{T} \right\} +$$

$$\frac{3}{4} A_2 \left[ \frac{2R_2 T}{U^2} \left( 1 + \frac{T^+}{T} \right) \frac{U^+}{U} \right] N_2^- N_2^+ \quad (2.10b)$$

Case 3.  $\epsilon_x^2$  - moment, rigid sphere gas

$$\frac{d}{d\xi} \left[ \frac{U^+}{U} N_1^+ \left\{ \frac{3R_1 T}{U^2} \left( \frac{T^+}{T} - 1 \right) - \left( 1 - \left( \frac{U^+}{U} \right)^2 \right) \right\} \right] =$$

$$- \frac{(2R_1 T)^{+3/2}}{U^3} \frac{1}{3 \sqrt{2K}} N_1^- N_1^+ \phi \left( \frac{U}{\sqrt{2R_1 T}} \frac{1 - U^+/U}{\sqrt{1 + T^+/T}} \right)$$

$$\left( 1 + \frac{T^+}{T} \right)^{3/2} - \frac{2R_1 T}{U^3} \frac{1}{\sqrt{2K}} \left( \frac{\beta}{1+\beta} \right)^2 \left( \frac{612}{\sigma} \right)^2$$

$$N_1^- N_2^+ \phi \left( \frac{U}{\sqrt{2R_1 T}} \frac{1 - U^+/U}{\sqrt{1 + \frac{1}{\beta} \frac{T^+}{T}}} \right),$$

$$\frac{1 + \beta}{\beta} \frac{1}{\left( 1 + \frac{T^+}{T} \frac{1}{\beta} \right)}, \frac{2(1 + \beta)}{\beta \left( 1 - \frac{U^+}{U} \right)} \left( 1 + \frac{T^+}{T} \frac{1}{\beta} \right)^{3/2}$$

$$- \frac{(2R_2 T)^{3/2}}{U^3} \frac{1}{\sqrt{2K}} \left( \frac{\beta}{1+\beta} \right)^2 \left( \frac{612}{\sigma} \right)^2 N_1^+ N_2^-$$

$$\phi \left( \frac{U}{\sqrt{2R_2 T}} \frac{1 - \frac{U^+}{U}}{\sqrt{1 + \frac{T^+}{T} \beta}} \right), \frac{T^+}{T} \frac{1 + \beta}{\left( \frac{T^+}{T} + \frac{1}{\beta} \right) \beta},$$

$$\left( \frac{-2 \frac{U^+}{U} (1 + \beta)}{(1 - \frac{U^+}{U}) \beta} \right) \left( 1 + \frac{T^+}{T} \beta \right)^{3/2} \quad (2.11a)$$

and

$$\begin{aligned}
 & \frac{d}{d\xi} \left\{ \frac{U^+}{U} N_2^+ \left[ \frac{3R_2 T}{U^2} \left( \frac{T^+}{T} - 1 \right) - \left( 1 - \left( \frac{U^+}{U} \right)^2 \right) \right] \right\} = \\
 & - \frac{(2R_2 T)^{3/2}}{U^3} \frac{1}{3\sqrt{2\pi}} \left( \frac{\sigma_{12}}{\sigma_1} \right)^2 N_2^- N_2^+ \cdot \\
 & \Theta \left( \frac{U}{\sqrt{2R_2 T}} \frac{1 - U^+/U}{\sqrt{1 + T^+/T}} \right) \left( 1 + \frac{T^+}{T} \right)^{3/2} \\
 & - \frac{(2R_2 T)^{3/2}}{U^3} \frac{1}{\sqrt{2\pi}} \left( \frac{\sigma_{12}}{\sigma_1} \right)^2 \frac{1}{(1+\beta)^2} \left( 1 + \frac{T^+}{T} \beta \right)^{3/2} \\
 & N_1^+ N_2^- * \Theta \left( \frac{U}{\sqrt{2R_2 T}} \frac{1 - U^+/U}{\sqrt{1 + (T^+/T)\beta}} \right), \frac{1 + \beta}{\frac{T^+}{T} \beta + 1}, \\
 & \frac{2(1 + \beta)}{1 + \frac{U^+}{U} \beta} \left) - \frac{(2R_1 T)^{3/2}}{U^3} \frac{1}{\sqrt{2\pi}} \left( \frac{\sigma_{12}}{\sigma_1} \right)^2 \\
 & \frac{1}{(1 + \beta)^2} \left( 1 + \frac{T^+}{T} \frac{1}{\beta} \right)^{3/2} N_1^- N_2^+ * \\
 & \Theta \left( \frac{U}{\sqrt{2R_1 T}} \frac{1 - U^+/U}{\sqrt{1 + \frac{T^+}{T} \frac{1}{\beta}}} \right), \frac{(T^+/T)(1 + \beta)}{(\beta + T^+/T)}, \\
 & \frac{-2 \frac{U^+}{U} (1 + \beta)}{1 - \frac{U^+}{U}} \left) \right. \quad (2.11b)
 \end{aligned}$$

where  $\Theta$  and  $\phi$  are the same functions as defined in Chapter I.

(2.11b)

Each of the system (2.9), (2.10) and (2.11) consists of a first order nonlinear, coupled differential equations and is subject to the following boundary conditions.

$$\begin{aligned} \text{As } \xi \rightarrow +\infty, \quad N_1^+ &\rightarrow \frac{1}{\xi} \\ N_2^+ &\rightarrow \frac{\infty}{\xi} \end{aligned} \quad (2.12a)$$

The solution is physically acceptable, if at the other end, i.e.,  $\xi \rightarrow -\infty$ , it satisfies

$$\lim_{\xi \rightarrow -\infty} N_1^+ = 0, \quad \lim_{\xi \rightarrow -\infty} N_2^+ = 0 \quad (2.12b)$$

It appears that we may start the integration from either end and verify that the conditions at the other end are fulfilled. However, in practice, the procedure is not as straight forward as it seems; one can start integration from only that end which satisfies the criterion for being a 'saddle point.' This point will be elaborated in the following. The detailed discussion will be given for the system (2.9).

### Theory:

To analyse such differential systems which are autonomous (because there is no explicit dependence of independent variable on slope function) phase plane-methods are used. The singular points are located and the behaviour of the integral curves in the neighbourhood of the singu-

lar points are examined. The knowledge of the nature of singular point and the slope functions enables one to predict the qualitative features of the system.

For example, let us consider the system.

$$\begin{aligned}\frac{dX}{d\xi} &= a_{11}X + a_{12}Y \\ \frac{dY}{d\xi} &= a_{21}X + a_{22}Y\end{aligned}\tag{2.13}$$

This system is autonomous because there is no  $\xi$ -dependence on the right hand side. Moreover  $Y = X = 0$  is a singular point because both the slope functions vanishes for these values of  $X$  and  $Y$ . Looking for solution in the  $(X, Y)$  plane, we write as

$$\frac{dY}{dX} = \frac{a_{21}X + a_{22}Y}{a_{11}X + a_{12}Y}\tag{2.14}$$

It is possible to start the integration of (2.14) if we know the starting slope  $\delta$ , where  $\delta$  is the limit, as the singular point is reached, of the ratio  $Y/X$ .

The procedure to calculate  $\delta$  consists of first solving the following algebraic equation (in an unknown  $\lambda$  - nothing to do with the mean free path)

$$\begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = 0$$

If the values of  $\lambda$  are real and of opposite signs, the

singular point is classified as 'saddle point'. If the values of  $\lambda$ , are real and of same sign it is classified as 'node'. When the singular point is saddle there are only four integral curves passing through the point and the selection of one of them which is relevant to the problem becomes possible.

Gilbarg (1951) applied this method to study the shock wave structure in a single gas using the continuum theory and proved that in the single gas case, as long as the gas satisfies a certain (fairly liberal) equation of state, the downstream singularity is saddle and the upstream one is node in character.

However, we shall show here below that such a general result is not available for our (mixture) problem; the nature of the singular points depends on the set of values of  $(OC, \beta, M)$ . We start with the singular point at the downstream infinity.

#### Downstream infinity:

Here

$$X = -\frac{1}{\epsilon} + N_1^+$$

$$Y = -\frac{OC}{\epsilon} + N_2^+$$

so that the linearised form of the equations (2.9 a-b), valid in the neighbourhood of this point, are

$$\frac{d}{d\zeta} \begin{pmatrix} X \\ Y \end{pmatrix} = \mathbf{a} \begin{pmatrix} X \\ Y \end{pmatrix}$$

where

$$a_{11} = (r_1 q_2 - r_2 q_1) / (p_1 q_2 - p_2 q_1)$$

$$a_{12} = (s_1 q_2 - s_2 q_1) / (p_1 q_2 - p_2 q_1)$$

$$a_{21} = (p_1 r_2 - p_2 r_1) / (p_1 q_2 - p_2 q_1)$$

$$a_{22} = (p_1 s_2 - p_2 s_1) / (p_1 q_2 - p_2 q_1)$$

and

$$p_2 = \frac{1}{4} \frac{5R_1^T}{U^2} \frac{\alpha^2 (\beta - 1)}{(1 + \alpha\beta)^2} \left[ \frac{3R_2^T}{U^2} (\epsilon - 1) - (1 - \epsilon^2) \right] \\ - \frac{1}{2} \frac{3R_2^T}{U^2} \frac{\alpha^2 \epsilon^2}{1 + \alpha\epsilon} \frac{(\beta - 1)}{(1 + \alpha\beta)} - \frac{3}{5\beta} \\ \frac{\alpha^2 \epsilon (\beta - 1) (1 - \epsilon^2)}{(1 + \alpha\epsilon)^2} + \frac{1}{2} \frac{5R_1^T}{U^2} \frac{\alpha^2 \epsilon^2 (\beta - 1)}{(1 + \alpha\beta)^2}$$

$$q_2 = \left( \frac{1}{4} \frac{5R_1^T}{U^2} \frac{(1 - \beta) \alpha}{(1 + \alpha\beta)^2} + \epsilon \right) \left[ \frac{3R_2^T}{U^2} (\epsilon - 1) - (1 - \epsilon^2) \right] \\ + \frac{3R_2^T}{U^2} \frac{\alpha}{1 + \alpha\epsilon} \epsilon (\beta - 1) \left[ \frac{1}{2(1 + \alpha\beta)} + \frac{U^2}{5R_1^T} \frac{(1 - \epsilon^2)}{(1 + \alpha\epsilon)} \right] \\ + \frac{1}{2} \frac{5R_1^T}{U^2} \frac{\alpha \epsilon^2 (1 - \beta)}{(1 + \alpha\beta)^2}$$

$$r_2 = \left[ \frac{1}{4} \frac{5R_1^T}{U^2} \frac{\alpha^2 (\beta - 1) (1 - \epsilon)^2}{(1 + \alpha\beta)^2} - \alpha \epsilon (1 - \epsilon) - \frac{R_1^T}{U^2} \frac{(\epsilon - 1)}{(1 + \beta)} \right] \frac{4A_1}{1 + \beta} x_{12} - \frac{(4A_1 - 2A_2)}{(1 + \beta)^2}$$

$$\alpha (1 - \epsilon)^2 \left( 1 + \frac{1}{2} \frac{5R_1 T}{U^2} - \frac{1}{\epsilon} \frac{\alpha (\beta - 1)}{(1 + \alpha \beta)^2} \right)$$

$$+ x_{22} A_2 \frac{\alpha^3}{\epsilon} (1 - \epsilon)^2 \frac{1}{4} \frac{5R_1 T}{U^2} \frac{(\beta - 1)}{(1 + \alpha \beta)^2}$$

$$s_2 = \left[ \frac{1}{4} \frac{5R_1 T}{U^2} - \frac{(1 - \beta) \alpha \epsilon}{(1 + \alpha \beta)^2} \left( \frac{1 - \epsilon}{\epsilon} \right)^2 + \epsilon - 1 - \right.$$

$$\left. \frac{R_1 T}{U^2} \frac{\epsilon - 1}{1 + \beta} \right] \frac{4A_1}{1 + \beta} x_{12} - \frac{(4A_1 - 2A_2)}{(1 + \beta)^2} (1 - \epsilon)^2$$

$$\left( 1 + \frac{2\alpha}{\epsilon} - \frac{1}{4} \frac{5R_1 T}{U^2} \frac{(1 - \beta) \epsilon}{(1 + \alpha \beta)^2} \right) + x_{22} A_2 \frac{\alpha}{\epsilon}$$

$$(1 - \epsilon)^2 * \left( \epsilon + \frac{\alpha}{\epsilon} - \frac{1}{4} \frac{5R_1 T}{U^2} \frac{(1 - \beta) \epsilon}{(1 + \alpha \beta)^2} \right)$$

$$p_1 = \left( \epsilon + \frac{1}{4} \frac{5R_1 T}{U^2} \frac{\alpha (\beta - 1)}{(1 + \alpha \beta)^2} \right) \left[ \frac{3R_1 T}{U^2} (\epsilon - 1) - \right.$$

$$\left. (1 - \epsilon^2) \right] + \frac{3R_1 T}{U^2} \left( - \frac{1}{2} \frac{\alpha (\beta - 1) \epsilon^2}{(1 + \alpha \beta)^2} - \frac{U^2}{5R_1 T} \right.$$

$$\left. \frac{\alpha (\beta - 1) \epsilon (1 - \epsilon^2)}{(1 + \alpha \beta)^2} + \frac{1}{2} \frac{5R_1 T}{U^2} \frac{\alpha (\beta - 1) \epsilon^2}{(1 + \alpha \beta)^2} \right)$$

$$q_1 = \frac{1}{4} \frac{5R_1 T}{U^2} \frac{(1 - \beta)}{(1 + \alpha \beta)^2} \left[ \frac{3R_1 T}{U^2} (\epsilon - 1) - (1 - \epsilon^2) \right]$$

$$+ \frac{3R_1 T}{U^2} \left( - \frac{1}{2} \frac{\epsilon (1 - \beta)}{(1 + \alpha \beta)^2} - \frac{U^2}{5R_1 T} \right.$$

$$\left. \frac{\epsilon (1 - \beta) (1 - \epsilon^2)}{(1 + \alpha \beta)^2} \right) + \frac{1}{2} \frac{5R_1 T}{U^2} \frac{(1 - \beta) \epsilon^2}{(1 + \alpha \beta)^2}$$

$$\begin{aligned}
r_1 = & x_{12} \frac{4A_1\beta}{1+\beta} \left\{ \frac{1}{4} \frac{5R_1T}{U^2} \frac{\alpha^2(\beta-1)(1-\epsilon)^2}{\epsilon(1+\alpha\beta)^2} + \right. \\
& \left. \alpha(1-\epsilon) + \frac{\alpha R_1T}{U^2} \frac{(\epsilon-1)}{(1+\beta)} \right\} - x_{12} (4A_1 - 2A_2) * \\
& \left( \frac{\beta}{1+\beta} \right)^2 (1-\epsilon)^2 \left\{ \alpha + \frac{1}{2} \frac{5R_1T}{U^2} \frac{\alpha^2(\beta-1)}{\epsilon(1+\alpha\beta)^2} \right\} + \\
& \frac{A_2}{\epsilon} (1-\epsilon)^2 \left( \epsilon + \frac{1}{4} \frac{5R_1T}{U^2} \frac{\alpha(\beta-1)\epsilon}{(1+\alpha\beta)^2} \right) \\
s_1 = & -x_{12} \frac{4A_1\beta}{1+\beta} \left\{ (1-\epsilon) \left[ \frac{(1-\epsilon)(\beta-1)\alpha}{\epsilon(1+\alpha\beta)^2} * \right. \right. \\
& \left. \left. \frac{1}{4} \frac{5R_1T}{U^2} + \epsilon \right] - \frac{R_1T}{U^2} (\epsilon-1) \frac{1}{(1+\beta)} \right\} - x_{12} (4A_1 - 2A_2) \\
& \left( \frac{\beta}{1+\beta} \right)^2 (1-\epsilon)^2 * \left\{ 1 + \frac{1}{2} \frac{5R_1T}{U^2} \frac{\alpha(1-\beta)}{\epsilon(1+\alpha\beta)^2} \right\} + \\
& \frac{A_2}{\epsilon} (1-\epsilon)^2 \frac{1}{4} \frac{5R_1T}{U^2} \frac{(1-\beta)}{(1+\alpha\beta)^2}
\end{aligned}$$

The roots of the characteristic equation are  $\lambda_1$  and  $\lambda_2$  which satisfy

$$\begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = 0$$

The values of  $\lambda_1, \lambda_2$  for various values of the set of parameter  $(\alpha, \beta, M)$  are given in the table I. It is



observed that in only a few cases is this end a saddle. For such set of values of  $(OC, \beta, M)$  integration may be started from this end. For others we have to examine the nature of the upstream infinity.

### Upstream Infinity:

Here we do not need to define new  $X$  and  $Y$  as  $N_1^+$  and  $N_2^+$  themselves vanish at this singular point. However, one cannot obtain directly the linear form (2.13) of the equations (2.9) because of the repeated occurrence of the expression  $\frac{N_1^+ + N_2^+}{N_1^+ + \beta N_2^+}$  (which is of the form  $0/0$  at the singular point) and its derivative.

$$\text{If limit } \lim_{\xi \rightarrow -\infty} \frac{N_2^+}{N_1^+} = \delta$$

$$\text{then } \lim_{\xi \rightarrow -\infty} \frac{U^+}{U} = \frac{1}{4} \left( 1 + \frac{5R_1 T}{U^2} \frac{1 + \delta}{1 + \beta \delta} \right) = V^* \text{ (say)}$$

$$\lim_{\xi \rightarrow -\infty} \frac{T^+}{T} = 1 + \frac{U^2}{5R_1 T} \frac{1 + \beta \delta}{1 + \delta} \left[ \frac{15}{16} - \frac{1}{16} \left( \frac{5R_1 T}{U^2} \right)^2 \right]$$

$$\left[ \frac{(1 + \delta)^2}{(1 + \beta \delta)^2} - \frac{10}{16} \frac{R_1 T}{U^2} \frac{1 + \delta}{1 + \beta \delta} \right] = W^* \text{ (say)}$$

Consequently, when the system (2.9) is linearised with respect to  $N_1^+, N_2^+$  the elements of the coefficient matrix  $\underline{a}$  will contain  $\delta$ , in addition to  $OC, \beta, M$ . The final linearised form is

$$\frac{d}{d\xi} \begin{pmatrix} N_1^+ \\ N_2^+ \end{pmatrix} = b \begin{pmatrix} N_1^+ \\ N_2^+ \end{pmatrix}$$

where

$$b_{11} = V_*^{-1} \left[ \frac{3R_1 T}{U^2} (\mathbb{W}^* - 1) - (1 - V_*^{*2}) \right]^{-1}$$

$$\left[ x_{12} \frac{4A_1 \beta}{1 + \beta} \propto V^* (1 - V^*) - x_{12} \frac{4A_1 \beta}{1 + \beta} \right. \\ \left. \propto \frac{R_1 T}{U^2 (1 + \beta)} (\mathbb{W}^* - 1) + x_{12} (4A_1 - 2A_2) \left( \frac{\beta}{1 + \beta} \right)^2 \right. \\ \left. \propto (1 - V^*)^2 - A_2 (1 - V^*)^2 \right] \equiv a(\delta)$$

$$b_{12} = V_*^{-1} \left[ \frac{3R_1 T}{U^2} (\mathbb{W}^* - 1) - (1 - V_*^{*2}) \right]^{-1}$$

$$\left[ x_{12} \frac{4A_1 \beta}{1 + \beta} (V^* - 1) + x_{12} \frac{4A_1 \beta}{1 + \beta} \frac{R_1 T}{U^2} (\mathbb{W}^* - 1) + \right. \\ \left. x_{12} (4A_1 - 2A_2) \left( \frac{\beta}{1 + \beta} \right)^2 (1 - V^*)^2 \right] \equiv b(\delta)$$

$$b_{21} = V_*^{-1} \left[ \frac{3R_2 T}{U^2} (\mathbb{W}^* - 1) - (1 - V_*^{*2}) \right]^{-1}$$

$$\left[ x_{12} \frac{4A_1 \beta}{1 + \beta} \propto (V^* - 1) + x_{12} \frac{4A_1}{(1 + \beta)} \propto \frac{R_1 T}{U^2} (\mathbb{W}^* - 1) \right. \\ \left. + \frac{\propto x_{12} (4A_1 - 2A_2)}{(1 + \beta)^2} (1 - V^*)^2 \right] \equiv c(\delta)$$

$$b_{22} = V_*^{-1} \left[ \frac{3R_2 T}{U^2} (\mathbb{W}^* - 1) - (1 - V_*^{*2}) \right]^{-1}$$

$$\left[ x_{12} \frac{4A_1}{1 + \beta} V^* (1 - V^*) + x_{12} \frac{4A_1}{(1 + \beta)^2} \frac{R_1 T}{U^2} (\mathbb{W}^* - 1) \right]$$

$$+ \frac{x_{12}(4A_1 - 2A_2)}{(1 + \beta^2)^2} * (1 - v^*)^2 - x_{22} A_2 \alpha (1 - v^*)^2 \Big] \equiv d(\delta)$$

Eigen values of the coefficient matrix are given by

$$\lambda_1, \lambda_2 = \frac{1}{2} (a(\delta) + d(\delta)) \pm \frac{1}{2} \left[ \{a(\delta) - d(\delta)\}^2 + 4b(\delta) c(\delta) \right]^{1/2}$$

As the roots  $\lambda_1, \lambda_2$  of the characteristic equation of  $b$  involve  $\delta$ , one cannot determine their sign from the knowledge of  $\alpha, \beta, K$  only; one has to solve for  $\delta$  from other consideration and then come back to determine the sign of  $\lambda$ 's. We proceed as follows:

Assume (to be verified a posteriori) that the upstream infinity is a saddle. Then  $\delta$  is determined as solution of the algebraic system

$$\delta = \frac{c(\delta)}{a(\delta) - \lambda_1(\delta)} \quad \text{or}$$

$$\delta = \frac{c(\delta)}{a(\delta) - \lambda_2(\delta)}$$

This algebraic system admits a finitely large number of solutions but the one satisfying the inequality

$$-\frac{a(\delta)}{b(\delta)} < \delta < \frac{-c(\delta)}{d(\delta)}$$

or

$$\frac{-c(\delta)}{d(\delta)} < \delta < \frac{-a(\delta)}{b(\delta)} \quad \text{is the one we seek.}$$

This leads to the following conclusion for system (2.9) expressed in the form:

$$\frac{dN_1^+}{dZ} = f(N_1^+, N_2^+)$$

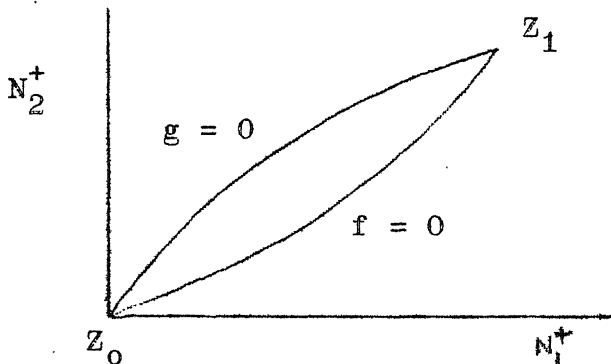
$$\frac{dN_2^+}{dZ} = g(N_1^+, N_2^+)$$

Firstly if there are only two solutions of the system

$$i) \quad g(N_1^+, N_2^+) = 0$$

$$f(N_1^+, N_2^+) = 0$$

Let us denote them by  $Z_0, Z_1$



ii) For a fixed  $N_1^+$  in the interval

$$0 \leq \bar{N}_1^+ \leq \frac{1}{\epsilon}$$

$$r \gg s$$

Where  $g(N_1^+, r) = 0$  and

$$f(N_1^+, s) = 0$$

iii) In the region bounded by the curves

$$g_{N_2^+} > 0$$

$$f_{N_2^+} < 0$$

iv) The point  $Z_0$  is saddle in character  
and (v) There is only one curve having direction  $\delta$  at  
the saddle point which satisfies the inequality

$$\frac{-f_{N_1^+}}{f_{N_2^+}} < \delta < \frac{-g_{N_1^+}}{g_{N_2^+}}$$

Then there exists an integral curve joining  $Z_0$  and  $Z_1$  which  
satisfies the differential equations and is unique.

For such values of the set  $(\alpha, \beta, M)$  which make  
the upstream singularity a saddle point, integration is  
started from upstream end. There are values of the set  
 $(\alpha, \beta, M)$  for which neither upstream nor downstream  
happens to be a saddle and the corresponding solution  
cannot be obtained by the systematic procedure. Here  
one has to resort to a guessing procedure, i.e., assume  
the values of  $N_2^+$  at a station (say  $\xi = 0$ ,  $N_1^+ = a$  where  
 $0 < a < \frac{1}{\epsilon}$ ; in particular  $N_1^+$  was taken to be equal to  
0.5 for numerical integration) and integrate in both direct-  
ions, i.e. towards  $-\infty$  and  $+\infty$ . If the boundary condi-  
tions are not satisfied, change the assumed value of  
 $N_2^+$  and repeat the process till a reasonable integral

curve is obtained. We have obtained solutions for three set of values of  $(\alpha, \beta, M)$  by this guessing procedure.

### Discussion:

A shock wave passing through a homogeneous gas mixture induces separation of species, i.e., the concentration of species changes in the shock wave. In the present context we shall not use the term first and second species and concentration ratio will denote the ratio of the number density of heavy species to the number density of light species and relative concentration ratio will be defined as the ratio of concentration ratio to initial concentration ratio. In order to bring out

- a) The effect of initial concentration ratio  $\alpha$ , mass ratio  $\beta$  and freestream Mach number  $M$  on the shock structure,
- b) A consistent trend, if any, in the  $c_x^2$  and  $c_x^3$  moment solutions and
- c) the effect of molecular model on the shock structure - the computation of number density profiles was carried out covering a good range of concentration ratio, mass ratio and freestream Mach number. The results have been presented graphically in Figs. 3 - 30 and are discussed below:

### Effect of concentration ratio:

The result of computation corresponding to  $\beta = 10$ ,  $M = 2$  and  $\alpha$  ranging from .022 to 2.5 has been reported in Figs. 3 - 6, 9 - 13, 15 and that of corresponding to  $\beta = 10$ ,

$M = 3$  and  $\alpha$  ranging from 2.0 to 3.0 has been reported in Figs. 19 - 21.

It is seen in these figures that the relative density curves do not intersect below a certain value of concentration ratio for a given mass ratio and free-stream Mach number. Thus, there seems to exist a critical concentration ratio for given pair of species depending upon  $\beta$  and  $M$  such that for any concentration ratio greater than the critical value, relative concentration ratio assumes a value greater than unity. This can also be expressed as 'the velocity of the heavy species remains greater than that of the light species throughout the shock wave as long as the concentration ratio does not exceed the critical concentration ratio'. It can also be seen that for a given  $\beta$  and  $M$  the number density at which intersection occurs decreases with increase in the concentration ratio and the overall rate of compression of heavy species increases with concentration ratio.

Such a trend of density profile is not found in any of the earlier numerical investigations. Bird (1968) has not made any computation in the range where this trend can be observed. Goldman and Sirovich (1969) have made computations in this range and have found the velocity of the heavy species higher than that of the light species throughout the shock wave along with the velocity undershoot of light species. Center (1967) claims to have done the experiment

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in this range but neither density profiles beyond  $\alpha = .923$  have been presented nor any remark about the intersection of density profile has been made. The density profiles corresponding to  $\alpha = .923$ ,  $\beta = 10$  and  $M = 2.25$  have been reproduced in Fig. 5 along with Center's experimental result. Intersection of density profiles can be seen in these figures. The second source of qualitative information on this subject is the asymptotic analysis carried out by Harris and Bienkowski (1971). Using asymptotic arguments they have shown that there exists more than one length scale of transition depending on the limiting values of  $\alpha$ ,  $\beta$ ,  $M$  and their products. According to their analysis when each of  $\alpha$ ,  $\beta$  and  $M$  is of order one, the transition occurs on one scale, i.e., light and heavy species are strongly coupled and the dissipative mechanisms resulting from self and cross-collisions are of order unity. On the other hand, when both  $\alpha$  and  $(\alpha\beta)$  are large in the limiting case on the inner scale, heavy-heavy self collisional shock is formed and light species is constant to the zero order. The pattern resulting from Figs. 12 - 1 seems to be in conformity with the view point of Harris and Bienkowski on account of regular shift of the point of interaction of density profiles and regular increase in overall compression rate of Argon. Thus we conclude

a) velocity of the heavy species is not always higher than that of the light species throughout the shock wave,



b) the velocity of species decreases monotonically to their corresponding Rankine-Pugoniot values

and (c) the pattern emerging from rate of compression of individual species and region where the species are significantly compressed (e.g., the region of significant compression of heavy species may be different from the region of significant compression of light species) suggests transition on multiple scales and formation of shock within shock.

#### Effect of Mach number:

The density profiles corresponding to  $M = 2$  and  $M = 3$  have been given in figs. 9 and 18. The values of  $\beta$  and  $\beta_3$ , the additional moment and the molecular model are left unchanged and their details are given in these figures. It is seen that separation of species measured in terms of difference of their relative number density or, equivalent, the difference of reciprocal of their bulk velocities increases with increase of freestream Mach number. The figures also suggest that heavy species starts getting decelerate only after the light species has been compressed significantly. This trend persists in  $c_x^3$  moment solution also as can be seen from Fig. 27. Examination of Figs. 13 and 19 shows that critical concentration ratio increases with increase in Mach number.

### Effect of mass ratio:

The density profiles corresponding to  $\beta = 10$  and  $\beta = 2$  have been given in Figs. 11 and 17. The other parameters are common to these sets and are given in the figures. As expected, more dissimilarity in mass creates more separation between the species. Another aspect of the effect of mass ratio can be seen in figures 12 and 16. These figures imply that as the mass ratio increases, while other parameters are held constant, critical concentration ratio decreases. It is also observed that the effect of mass ratio is more pronounced than <sup>that</sup> of concentration ratio on the separation of species as can be seen from Figs. 24 and 27 in which the effect of decreasing the concentration ratio by a factor of 10 gets obviated by decreasing the mass ratio by a factor of 2.

### Effect of additional moment on solution:

Though the overall qualitative aspects of the solution do not change with the choice of additional moment, a sharp quantitative difference can be seen from Figs. 6 and 22.  $C_x^3$  moment solution gives lower critical concentration ratio and it gives poor agreement with available experimental results.

### Effect of molecular model on solution:

Figs. 29 and 6 can be compared for this purpose. In this case, compression of both the species for rigid sphere gas takes place at a lower rate, thereby, thickening the shock. Separation of species is greater in Maxwell molecule model. For rigid sphere gas, increase of Mach number increases separation between the species and delays the compression of heavy species in the beginning also, as can be seen in Fig. 30. It may be appropriate to point out that with Mott-Smith ansatz Maxwell molecule model yields better agreement with available experimental results.

### Effect of force constants:

The situation to discuss this would not have arisen had the traditional values of  $X_{12}$  - a force constant determined from data of diffusion coefficient (based on near-equilibrium experiment) and Chapman-Enskog theory (whose validity is questionable in strong-non-equilibrium situation) - yielded satisfactory results. Phenomenon exhibiting diffusive effects being more complicated than the phenomenon exhibiting viscous effects, numerical experiments were carried out to see the effect of  $X_{12}$  on density profiles. It so happened that the change of  $X_{12}$  from 1.385 to 1.0 improves agreement with all the three available experiments. The effect of change of  $X_{12}$  on density profile can

be seen in Figs. 6 and 7 which also suggests that increase of  $X_{12}$  increases the overall compression rate of heavy species.

#### Sensitivity of numerical scheme:

Though the numerical difficulties in obtaining the solution are enormous, it is interesting to note that the final result is almost insensitive to higher order integration scheme. First and 8th order integration schemes with variable step size were used to compare the density profiles and they have been reported in Figs. 13, 14 for  $\alpha = 2.0$ ,  $\beta = 10.0$  and  $M = 2$  and in the Figs. 7 and 8 for  $\alpha = 0.1$ ,  $\beta = 10$  and  $M = 2$ . It seems likely that the effect of higher order integration is counterbalanced by the round-off error resulting from lengthy and ill-conditioned numerical operations.

#### Comparison with experiments:

1 Comparison with experiments of Center (1967) and Muntz (1972) have been given in Figs. 3 - 5 which also contain the details. The agreement with Harnett and Muntz's experiment which corresponds to  $M = 1.58$ ,  $\beta = 10$ ,  $\alpha = 0.111$  is very good, as can be seen in Fig. 3. Figs. 4 and 5 present the comparison with Center's experiment which correspond to  $M = 2.07$ ,  $\beta = 10$  and  $\alpha = 0.022$  and  $M = 2.24$ ,  $\beta = 10$  and

$\alpha = 0.923$ . It is seen that in the former case separation of species is slightly overpredicted over a small interval and in the latter case the separation of species is underpredicted over a large part of the shock wave. In spite of the quantitative agreement with experiment not being very close, as seen in Fig. 5, it is only the present computation which agrees with experimental results as regards qualitative aspect of intersection of density curves.

### Conclusion:

Thus the numerical experiments carried out lead to the following conclusions:

- i) The  $c_x^2$  moment and the model of Maxwell molecule give the most satisfactory results.
- ii) Separation of species depends strongly on the model of molecules and the additional moment chosen, and
- iii) Intersection of density curves of heavy and light species depends on the concentration ratio, mass ratio and free stream Mach number. Patterns resulting from the variation of these parameters suggest that the formation of heavy-heavy self collisional shock on the inner scale and transition of light species on the outer scale is possible for a large number of cases characterised by the limiting values of these parameters. This trend is in fair agreement with the asymptotic analysis of Harris and Bienkowski (1971) and the experiment of Center (1967) (Fig.5) and is not found in earlier numerical investigations.

### CHAPTER III

The arbitrariness in the Mott-Smith method (namely, the choice of the extra moment) and the criterion first set up by Oberai (1967) to remove the arbitrariness was discussed in the introduction. We shall extend his work to the mixture problem. The problem will be formulated for arbitrary Mach number, keeping the extended Mott-Smith ansatz intact.

Thus, the postulated distribution functions are

$$f_i = N_0 \left\{ N_i^-(x) (2\pi R_i T)^{-3/2} \exp \left[ -\frac{(c - U_i)^2}{2R_i T} \right] + N_i^+(x) (2\pi R_i T^+(x))^{-3/2} \exp \left[ -\frac{(c - U^+(x))_i^2}{2R_i T^+(x)} \right] \right\}$$

$i = 1, 2$  (3.1. (a))  
(b))

and

$$\begin{aligned} \lim_{x \rightarrow -\infty} N_i^+ &= 0, \quad i = 1, 2 \\ N_1^- &= 1 \\ N_2^- &= \infty \end{aligned}$$

$$\lim_{x \rightarrow +\infty} N_i^- = 0, \quad i = 1, 2$$

Where, from the conservation equations

$$N_1^-(x) = 1 - \frac{U^+(x)}{U} N_1^+(x) \quad (3.2)$$

$$N_2^-(x) = \infty - \frac{U^+(x)}{U} N_2^+(x) \quad (3.3)$$

$$\frac{U^+(x)}{U} = \frac{1}{4} \left( 1 + \frac{5R_1 T}{U^2} \frac{N_1^+ + N_2^+}{N_1^+ + \beta N_2^+} \right) \quad (3.4)$$

$$\frac{T^+}{T} = 1 + \frac{U^2}{5R_1 T} \left[ 1 - \left( \frac{U^+}{U} \right)^2 \right] \frac{N_1^+ + \beta N_2^+}{N_1^+ + N_2^+} \quad (3.5)$$

leaving only the two functions  $N_1^+(x)$  and  $N_2^+(x)$  to be determined.

The genesis of the method is that the unknown functions  $N_1^+$  and  $N_2^+$  may be so determined that the equations

$$c_x \frac{\partial f_i}{\partial x} = J(f_i, f_1) + J(f_i, f_2) = C_i^* \quad (\text{say}) \quad i = 1, 2 \quad (3.6(a))$$

(b)

[where  $J(f_i, f_1)$  stands for  $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_i(c_i) f_1(c_1) - f_i(c_i) f_1(c_1) g b db de dc_1$  and  $J(f_i, f_2)$  stands for similar integral]

are satisfied in the least square sense; viz. such as would make minimum the following integral:

$$\int_{-\infty}^{\infty} dx \int dc \left[ \sum_{i=1,2} \left( c_x \frac{\partial f_i}{\partial x} - C_i^* \right)^2 \right] \quad (3.7)$$

$$= \int_{-\infty}^{\infty} dx \int dc \left[ \sum_{i=1,2} \left\{ \left( c_x \frac{\partial f_i}{\partial x} \right)^2 - 2 c_x \frac{\partial f_i}{\partial x} C_i^* + C_i^{*2} \right\} \right]$$

$$= \int_{-\infty}^{\infty} (I_1 + I_2 + I_3) dx$$



where

$$I_1 = \int \sum_{i=1,2} (c_x \frac{\partial f_i}{\partial x})^2 d\underline{c} \quad (3.8)$$

$$I_2 = - \left\{ \sum_{i=1,2} 2 c_x \frac{\partial f_i}{\partial x} c_i^* d\underline{c} \right. \quad (3.9)$$

$$I_3 = \int \sum_{i=1,2} c_i^{*2} d\underline{c} \quad (3.10)$$

With the form of  $f_i$  given in (3.1) the integral  $I_1$  and  $I_2$  can be evaluated for either (Maxwellian and hard sphere)molecular model. However  $I_3$  involves the integration of  $c_i^{*2}$  which, in general, is a gigantic task.

However, as pointed out by Oberai (1967), in the limit: upstream  $M \rightarrow \infty$ , the supersonic modes in  $f_i$  approach 'Dirac's' delta function and  $I_3$  can be evaluated analytically for the hard sphere model.

In this limit (ie,  $M \rightarrow \infty$ ) the relations (3.4) and (3.5) get simplified to

$$\frac{U^+}{U^-} = \frac{1}{4} \quad (3.11)$$

$$2R_1 T^+ = \frac{3}{8} \frac{N_1^+ + \beta N_2^+}{N_1^+ + N_2^+} \quad (3.12)$$

Moreover

$$N_1^+ (x) = 4(1 - N_1^-) \quad (3.13)$$

$$N_2^+ (x) = 4(\infty - N_2^-) \quad (3.14)$$

$$\frac{N_1^+ + \beta N_2^+}{N_1^+ + N_2^+} = \frac{1 + \alpha \beta - N_1^-(x) - \beta N_2^-(x)}{1 + \alpha - N_1^-(x) - N_2^-(x)} \quad (3.15)$$

and the  $f_i$  may be rewritten as

$$f_1(x, \underline{c}) = N_1^-(x) \delta(\underline{c} - \underline{1}) + 4(1 - N_1^-(x)) \left[ \frac{3}{8} \bar{\Lambda} \frac{1 + \alpha \beta - N_1^-(x) - \beta N_2^-(x)}{1 + \alpha - N_1^-(x) - N_2^-(x)} \right]^{-3/2} \exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{1} \right)^2 \frac{8}{3} \frac{1 + \alpha - N_1^-(x) - N_2^-(x)}{1 + \alpha \beta - N_1^-(x) - \beta N_2^-(x)} \right] \quad (3.16)$$

and

$$f_2(x, \underline{c}) = N_2^-(x) \delta(\underline{c} - \underline{1}) + 4(\alpha - N_2^-(x)) \left[ \frac{3}{8} \frac{\bar{\Lambda}}{\beta} \frac{1 + \alpha \beta - N_1^-(x) - \beta N_2^-(x)}{1 + \alpha - N_1^-(x) - N_2^-(x)} \right]^{-3/2} \exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{1} \right)^2 \frac{8\beta}{3} \frac{(1 + \alpha - N_1^-(x) - N_2^-(x))}{1 + \alpha \beta - N_1^-(x) - \beta N_2^-(x)} \right] \quad (3.17)$$

Writing Boltzmann equation corresponding to first gas

$$\underline{c} \cdot \underline{1} \frac{\partial f_1}{\partial \underline{x}} = J_{11}(f_1, f_2) + J_{12}(f_1, f_2) = C_1^* \quad (3.18)$$

$$= J_{11} \left( N_1^-(x) \delta(\underline{c} - \underline{1}), 4(1 - N_1^-(x)) \left[ \frac{3}{8} \bar{\Lambda} \frac{1 + \alpha \beta - N_1^-(x) - \beta N_2^-(x)}{1 + \alpha - N_1^-(x) - N_2^-(x)} \right]^{-3/2} \exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{1} \right)^2 \frac{8}{3} \frac{1 + \alpha - N_1^-(x) - N_2^-(x)}{1 + \alpha \beta - N_1^-(x) - \beta N_2^-(x)} \right] \right) +$$

$$J_{11} \left( 4(1 - N_1^-) \left[ \frac{3\pi}{8} \frac{1 + \alpha\beta - N_1^- - N_2^-}{1 + \alpha - N_1^- - N_2^-} \right] \right)^{-3/2}$$

$$\exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \frac{8}{3} \frac{1 + \alpha - N_1^- - N_2^-}{1 + \alpha\beta - N_1^- - \beta N_2^-} \right],$$

$$N_1^-(x) \delta(\underline{c} - \underline{i}) \Big) + J_{12} \left( N_1^-(x) \delta(\underline{c} - \underline{i}), \right. \\ \left. 4(\alpha - N_2^-(x)) \left[ \frac{3}{8} \frac{\pi}{\beta} \frac{1 + \alpha\beta - N_1^- - \beta N_2^-}{1 + \alpha - N_1^- - N_2^-} \right] \right)^{-3/2}$$

$$\exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \frac{8\beta}{3} \frac{1 + \alpha - N_1^- - N_2^-}{1 + \alpha\beta - N_1^- - \beta N_2^-} \right] \Big) +$$

$$J_{12} \left( 4(1 - N_1^-(x)) \left[ \frac{3\pi}{8} \frac{1 + \alpha\beta - N_1^- - \beta N_2^-}{1 + \alpha - N_1^- - N_2^-} \right] \right)^{-3/2}$$

$$\exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \frac{8}{3} \frac{1 + \alpha - N_1^- - N_2^-}{1 + \alpha\beta - N_1^- - \beta N_2^-} \right],$$

$$N_2 \delta(\underline{c} - \underline{i}) \Big)$$

The leading terms of the right hand side are,

$$- \left[ \delta(\underline{c} - \underline{i}) 4 N_1^-(x) (1 - N_1^-) \left[ \frac{3\pi}{8} \frac{1 + \alpha\beta - N_1^- - \beta N_2^-}{1 + \alpha - N_1^- - N_2^-} \right] \right)^{-3/2}$$

$$\int \exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \frac{8}{3} \frac{1 + \alpha - N_1^- - N_2^-}{1 + \alpha\beta - N_1^- - \beta N_2^-} \right]$$

$$g b_1 db_1 d\underline{c} d \underline{c}_1 \Big] - \left\{ \delta(\underline{c} - \underline{i}) 4 N_1^-(x) (\alpha - N_2^-(x)) \right. \\ \left. \right)^{-3/2}$$

$$\left[ \frac{3}{8} \frac{\pi}{\beta} \frac{1 + \alpha\beta - N_1^- - \beta N_2^-}{1 + \alpha - N_1^- - N_2^-} \right] \int \exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \right]$$

$$\frac{8\beta}{3} \frac{1 + \mathcal{C} - N_1^- - N_2^-}{1 + \mathcal{C}(\beta - N_1^- - \beta N_2^-)} \left\{ g b_{eq} db_{eq} d\epsilon d\epsilon_1 \right\}$$

denoting

$$A(x) = \frac{1 + \mathcal{C} - N_1^- - N_2^-}{1 + \mathcal{C}(\beta - N_1^- - \beta N_2^-)}$$

These integrals reduce to

$$\begin{aligned} & - \left[ \delta(\underline{v}) 4 N_1^- (1 - N_1^-) \left( \frac{3\pi}{8A} \right)^{-3/2} \left\{ \left( \frac{9}{8} + \frac{3}{8A(x)} \right) \times \right. \right. \\ & \times \int_0^{\sqrt{\frac{3}{2}}} e^{-A(x)t^2} dt - \frac{9}{8} \sqrt{\frac{3}{2}} \frac{e^{-A(x)\frac{3}{2}}}{A(x)} \left. \left. \right\} \frac{1}{2} \sqrt{\frac{3}{2}} \pi^2 \right. \\ & \frac{1}{A(x)} + \delta(\underline{v}) 4 N_1^- (\mathcal{C} - N_2^-) \left( \frac{3\pi}{8A\beta} \right)^{-3/2} \\ & \left. \frac{1}{2} \sqrt{\frac{3}{2}} \pi^2 \frac{\sigma_{eq}^2}{A\beta} \left[ \left\{ \frac{9}{8} + \frac{3}{8A\beta} \right\} \right. \right. \\ & \left. \left. \int_0^{\frac{3}{2}} e^{-A\beta\tau^2} d\tau - \frac{9}{8} \sqrt{\frac{3}{2}} \frac{e^{-A(x)\beta\frac{3}{2}}}{A(x)\beta} \right] \right] \end{aligned}$$

To write the above mentioned result, we note the following integral.

$$\int_0^\infty g^2 e^{-A(x)} \left( \frac{8}{3} g^2 + \frac{3}{2} \right) \sinh(4g A(x)) dg$$

$$= \sqrt{\frac{3}{2}} \frac{1}{4} \left[ \int_0^{\sqrt{\frac{3}{2}}} e^{-\frac{1}{2}(x)t^2} dt \left( \frac{9}{8} + \frac{3}{8A(x)} \right) - \frac{9}{8} \sqrt{\frac{3}{2}} \frac{e^{-A \cdot 3/2}}{A} \right]$$

Similarly for the second gas

$$\begin{aligned} \underline{c} \cdot \underline{i} \frac{\partial f_2}{\partial \underline{x}} &= J_{21}(f_2, f_1) + J_{22}(f_2, f_2) \quad (3.19) \\ &= J_{21} \left( N_2^- \delta(\underline{v}), 4(1 - N_1^-) \left( \frac{3\pi}{8A} \right)^{-3/2} \exp \left[ - \frac{8A}{3} \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \right] \right) \\ &+ J_{21} \left( 4(\infty - N_2^-) \left( \frac{3\pi}{8A\beta} \right)^{-3/2} \exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \frac{8A\beta}{3} \right], \right. \\ &N_1^-(x) \delta(\underline{v}) \Big) + J_{22} \left( N_2^- \delta(\underline{v}), 4(\infty - N_2^-) \left( \frac{3\pi}{8A\beta} \right)^{-3/2} \right. \\ &\exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \frac{8A\beta}{3} \right] \Big) + J_{22} \left( 4(\infty - N_2^-) \left( \frac{3\pi}{8A\beta} \right)^{-3/2} \right. \\ &\exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \frac{8A\beta}{3} \right], N_2^- \delta(\underline{c} - \underline{i}) \Big) \end{aligned}$$

The leading terms are

$$\begin{aligned} &- \delta(\underline{v}) \left[ 4 N_2^- (1 - N_1^-) \left( \frac{3\pi}{8A} \right)^{-3/2} \int \exp \left[ - \left( \underline{c}_1 - \frac{1}{4} \underline{i} \right)^2 \frac{8A}{3} \right] \right. \\ &\left. g b_{e,q} db_{e,q} d\underline{c} d\underline{c}_1 \right. \\ &+ 4N_2^- (\infty - N_2^-) \left( \frac{3\pi}{8A\beta} \right)^{-3/2} \int \exp \left[ - \left( \underline{c}_1 - \frac{1}{4} \underline{i} \right)^2 \frac{8\beta A}{3} \right] \\ &\left. g b_{e,q} db_{e,q} d\underline{c} d\underline{c}_1 \right] = - \delta(\underline{v}) \left\{ 4 N_2^- (1 - N_1^-) \left( \frac{3\pi}{8A} \right)^{-3/2} \right. \\ &\left. \frac{1}{2} \sqrt{\frac{3}{2}} \pi^2 \frac{6e_q}{A} \left[ \left( \frac{9}{8} + \frac{3}{8A} \right) \right] \right\} \end{aligned}$$

$$\int_0^{\sqrt{\frac{3}{2}}} e^{-A(x)t^2} dt - \frac{9}{8} \sqrt{\frac{3}{2}} \frac{e^{-A3/2}}{A} \Big] + 4N_2^- (\infty - N_2^-) +$$

$$\left( \frac{3\bar{A}}{8A\beta} \right)^{-3/2} \frac{1}{2} \sqrt{\frac{3}{2}} \bar{A}^2 \frac{\sigma_2^2}{A\beta} \left[ \left( \frac{9}{8} + \frac{3}{8A} \right) \int_0^{\sqrt{\frac{3}{2}}} e^{-A\beta t^2} dt - \right.$$

$$\left. \frac{9}{8} \sqrt{\frac{3}{2}} \frac{e^{-A\beta \cdot 3/2}}{A\beta} \right] \Big\}$$

Introducing a new function  $M(A)$ , defined as  $M(A)$

$$= 16 \sqrt{\frac{2}{3}} \bar{A} A \left[ \left( \frac{9}{8} + \frac{3}{8A} \right) \int_0^{\sqrt{3/2}} e^{-At^2} dt - \frac{9}{8} \sqrt{\frac{3}{2}} \frac{e^{-3A/2}}{A} \right]$$

the collision integral can be written as,

$$C_1^* = - \left[ N_1^- (1 - N_1^-) M(A) \sigma_1^2 + N_1^- (\infty - N_2^-) M(A\beta) \right. \\ \left. \sigma_{eq}^2 \right] \delta(\underline{v}) \quad (3.20)$$

$$C_2^* = - \left[ N_2^- (1 - N_1^-) M(A) \sigma_{eq}^2 + N_2^- (\infty - N_2^-) M(A\beta) \right. \\ \left. \sigma_2^2 \right] \delta(\underline{v}) \quad (3.21)$$

We want to determine  $N_1^-$  and  $N_2^-$  subject to minimization of the functional

$$\int \left[ \left\{ \underline{c} \cdot \underline{i} \frac{\partial f_1}{\partial \underline{x}} - C_1^* \right\}^2 + \left\{ \underline{c} \cdot \underline{i} \frac{\partial f_2}{\partial \underline{x}} - C_2^* \right\}^2 \right] d\underline{c} d\underline{x} \quad (3.22)$$

Noting

$$\underline{c} \cdot \underline{i} \frac{\partial f_1}{\partial \underline{x}} = u \frac{dN_1^-}{d\underline{x}} \delta(\underline{c} - \underline{i}) + u \frac{d}{d\underline{x}} \left\{ 4 (1 - N_1^-) \left( \frac{3\bar{A}}{8A} \right)^{-3/2} \right.$$

$$\left. \exp \left[ - \left( \underline{c} - \frac{1}{4} \underline{i} \right)^2 \frac{8A}{3} \right] \right\}$$

$$\begin{aligned}
\int \left\{ c, i \frac{\partial f_1}{\partial x} \right\}^2 d c &= \left( \frac{dN_1^-}{dx} \right)^2 \left( \frac{5}{12\pi} \right)^{3/2} \left( \frac{1 + \alpha}{1 + \alpha\beta} \right)^{3/2} M^3 + o(M^2) \\
\int c, i \frac{\partial f_1}{\partial x} C_1^* d c &= - \left( \frac{5}{12} \right)^{3/2} \left( \frac{1 + \alpha}{1 + \alpha\beta} \right)^{3/2} M^3 \frac{dN_1^-}{dx} \\
&\left[ N_1^- (1 - N_1^-) M(A) + N_1^- (\alpha - N_2^-) M(A\beta) \right] + o(M^2) \\
\int C_1^{*2} d c &= \left[ N_1^- (1 - N_1^-) M(A) + N_1^- (\alpha - N_2^-) M(A\beta) \right]^2 \times \\
&\left( \frac{5}{12} \right)^{3/2} \left[ \frac{1 + \alpha}{1 + \alpha\beta} \right]^{3/2} M^3 + o(M^2)
\end{aligned}$$

Finally it amounts to minimizing the integral

$$\begin{aligned}
&\int \left\{ \left[ \left( \frac{dN_1^-}{dx} \right)^2 + 2 \frac{dN_1^-}{dx} \left[ N_1^- (1 - N_1^-) M(A) + N_1^- (\alpha - N_2^-) M(A\beta) \right] \right. \right. \\
&\quad \left. \left. + \left[ N_1^- (1 - N_1^-) M(A) + N_1^- (\alpha - N_2^-) M(A\beta) \right]^2 \right\} + \left\{ \left( \frac{dN_2^-}{dx} \right)^2 + \right. \right. \\
&\quad \left. \left. 2 \frac{dN_2^-}{dx} \left[ N_2^- (1 - N_1^-) M(A) + N_2^- (\alpha - N_2^-) M(A\beta) \right] + \right. \right. \\
&\quad \left. \left. \left[ N_2^- (1 - N_1^-) M(A) + N_2^- (\alpha - N_2^-) M(A\beta) \right]^2 \right\} \right\} dx \quad (3.23)
\end{aligned}$$

This yields the following equations,

$$\begin{aligned}
&\frac{d}{dx} \left\{ \frac{dN_1^-}{dx} + \left[ N_1^- (1 - N_1^-) M(A) + N_1^- (\alpha - N_2^-) M(A\beta) \right] \right\} \\
&= \frac{dN_1^-}{dx} \left[ (1 - 2N_1^-) M(A) + N_1^- (1 - N_1^-) M'(A) \frac{\partial A}{\partial N_1^-} + \right. \\
&\quad \left. (\alpha - N_2^-) M(A\beta) + N_1^- (\alpha - N_2^-) M'(A\beta) \beta \frac{\partial A}{\partial N_1^-} \right] + \\
&\frac{dN_2^-}{dx} \left[ N_2^- (1 - N_1^-) M'(A) \frac{\partial A}{\partial N_2^-} - N_2^- M(A) + N_2^- (\alpha - N_2^-) \right. \\
&\quad \left. M'(A\beta) \beta \frac{\partial A}{\partial N_1^-} \right] + \left[ N_1^- (1 - N_1^-) M(A) + N_1^- (\alpha - N_2^-) \right. \\
&\quad \left. M(A\beta) \right] \times
\end{aligned}$$

$$\begin{aligned} & \left[ (1 - 2N_1^-) M(A) + N_1^- (1 - N_1^-) M^I(A) \frac{\partial A}{\partial N_1^-} (\infty - N_2) M(A\beta) + \right. \\ & N_1^- (\infty - N_2^-) M^I(A\beta) \beta \frac{\partial A}{\partial N_1^-} \left. \right] + \left[ N_2^- (1 - N_1^-) M(A) + \right. \\ & N_2^- (\infty - N_2^-) M(A\beta) \left. \right] - \left[ N_2^- (1 - N_1^-) M^I(A) \frac{\partial A}{\partial N_1^-} + \right. \\ & N_2^- M(A) + N_2^- (\infty - N_2^-) M^I(A\beta) \beta \frac{\partial A}{\partial N_1^-} \left. \right] \quad (3.24a) \end{aligned}$$

and

$$\begin{aligned} & \frac{d}{dx} \left[ \frac{dN_2^-}{dx} + N_2^- (1 - N_1^-) M(A) + N_2^- (\infty - N_2^-) M(A\beta) \right] = \\ & \frac{dN_2^-}{dx} \left[ (1 - N_1^-) M(A) + N_2^- (1 - N_1^-) M^I(A) \frac{\partial A}{\partial N_2^-} + \right. \\ & (\infty - 2N_2^-) M(A\beta) + N_2^- (\infty - N_2^-) M^I(A\beta) \frac{\partial A}{\partial N_2^-} \left. \right] + \\ & \frac{dN_1^-}{dx} \left[ N_1^- (1 - N_1^-) M^I(A) \frac{\partial A}{\partial N_2^-} - N_1^- M(A\beta) + N_1^- (\infty - N_2^-) \right. \\ & M^I(A\beta) \beta \frac{\partial A}{\partial N_2^-} \left. \right] + \left[ N_2^- (1 - N_1^-) M(A) + N_2^- (\infty - N_2^-) \right. \\ & M(A\beta) \left. \right] \left[ (1 - N_1^-) M(I) + N_2^- (1 - N_1^-) M^{II}(A) \right. \\ & \frac{\partial A}{\partial N_2^-} + (\infty - 2N_2^-) M(A\beta) + N_2^- (\infty - N_2^-) M^{II}(A\beta) \\ & \left. \beta \frac{\partial A}{\partial N_2^-} \right] + \left[ N_1^- (1 - N_1^-) M(A) + N_1^- (\infty - N_2^-) M(A\beta) \right] \\ & \left[ N_1^- (1 - N_1^-) M^I(A) \frac{\partial A}{\partial N_2^-} + N_1^- (\infty - N_2^-) M^I(A\beta) \beta \frac{\partial A}{\partial N_2^-} - \right. \\ & N_1^- M(A\beta) \left. \right] \quad (3.24b) \end{aligned}$$



These equations have to be solved subject to the following boundary conditions:

$$\begin{aligned} \lim_{x \rightarrow \infty} N_1^- &= 0, \quad i = 1, 2 \\ \lim_{x \rightarrow -\infty} N_1^- &= 1 \\ N_2^- &= \infty \end{aligned} \quad 3.24(c)$$

The system (3.24) is far more complicated than that encountered in Chapter II. What we have gained in terms of freedom from arbitrariness is more than offset by the almost unmanageable complexity of the (differential) system to be solved.

For a few typical cases the numerical solutions obtained by three-fold guessing (i.e. at  $x = 0$ , one chooses a reasonable value of  $N_1^-$ , say 0.5, and guesses the corresponding values of  $N_2^-$ ,  $\frac{dN_1^-}{dx}$ ,  $\frac{dN_2^-}{dx}$  that lead to correct behaviour at  $\pm \infty$ ) are given in Fig. (31) and (32b).

In conclusion, it may be mentioned that for the bimodal function (i.e. for the single gas problem) Narasimha and Deshpande (1969) have succeeded in evaluating, in closed form, the collision integral  $J$ , for the hard sphere molecular model. However, the related integrals appearing as co-efficients in Euler's equation does not depend on position and this simplicity is lost in the corresponding problem for the gaseous mixture and the problem remains untractable.

APPENDIX.

Two particles of masses  $m_1$  and  $m_2$  moving with velocities  $\underline{c}_1$  and  $\underline{c}_2$  collide  $\underline{c}_1'$  and  $\underline{c}_2'$  are their final velocities. The initial relative velocity is deviated by  $\underline{g}$  and  $\underline{j}$  is the unit vector along the direction joining the position of the particle  $m_1$  and the point of intersection of the asymptotes to the trajectory, describing the relative motion of  $m_2$  (Fig. (1a)).

Then (cf. Ref. (8), Sec. 3.43, Chapman and Cowling (1964))

$$\underline{c}_1' - \underline{c}_1 = 2(m_2/(m_1 + m_2)) (\underline{g}, \underline{j}) \underline{j}$$

$$\underline{c}_2' - \underline{c}_2 = -2(m_1/(m_1 + m_2)) (\underline{g}, \underline{j}) \underline{j}$$

Again (see Fig. 1(b))

$$\underline{i}, \underline{j} = \cos \theta \cos \psi + \sin \theta \sin \psi \cos \phi$$

therefore

$$u_1' - u_1 = (\underline{c}_1' - \underline{c}_1) \cdot \underline{i}$$

$$= 2 \frac{m_2}{(m_1 + m_2)} g \cos \theta (\cos \theta \cos \psi + \sin \theta \sin \psi \cos \phi)$$

$$u_2' - u_2 = -2 \frac{m_1}{m_1 + m_2} g \cos \theta (\cos \theta \cos \psi + \sin \theta \sin \psi \cos \phi)$$

$$\text{Also } \cos \psi = (u_2 - u_1)/g$$

and the angle of deflection  $\chi = \pi - 2\theta$

Calculation of

$\int \phi(\underline{c}) J(f, f) d\underline{c}$  for Maxwell molecule require  
evaluation of

$$\int_0^{\infty} (1 - \cos^l \chi) v_0 dv_0 \quad \text{denoted by } A_1$$

which has been taken from Chapman and Cowling (1964) and  
Mott-Smith (1954).

TABLE - I  
DOWNSTREAM SINGULAR POINT EIGENVALUES  $\lambda_1$  and  $\lambda_2$

M		$\beta$				
		2	10	20	50	100
2	$\infty$					
	100	-0.9763 -01.4444	-0.3409 -0.9814	-0.1773 -0.9832	-0.0726 -0.9888	-0.0365 -0.9974
2	10	-01.002	-0.3386	-0.1763	-0.0736	-0.0393
	02	-01.512	-1.1000	-1.1268	-1.1808	-1.2324
2	10	-1.0996	-0.3638	-0.2040	-0.1032	-0.0686
	10	-1.8314	-1.6150	-1.7713	-2.2672	-3.7872
2	10	-1.9480	3.9519	1.4247	0.4836	0.2285
	10	3.3082	-1.0334	-0.8571	-0.7479	-0.7136
2	10	179.842	4.5159	2.0287	0.7619	0.3730
	10	-9.7233	-9.7419	-8.5735	-8.4716	-8.4381
2	100	832.7173	34.2951	15.5166	5.8534	2.8702
	100	-86.9460	-85.9564	-85.7885	-85.6858	-85.6516

TABLE - I (contd)  
DOWNSTREAM SINGULAR POINT EIGENVALUES  $\lambda_1$  AND  $\lambda_2$

M	$\infty$	2	10	20	50	100
5	.001	-2.1925	-.5974	-.3120	-.1287	-.0653
		-2.4870	-2.1975	-2.1982	-2.1995	-2.2013
5	.02	-2.2440	-.6213	-.3313	-.1452	-.0810
		-2.6067	-2.3500	-2.3650	-2.3943	-2.4317
5	.10	-2.4368	-.7341	-.4271	-.2302	-.1636
		-3.1610	-3.1188	-3.3417	-4.1229	-6.6440
5	1.0	-4.3170	6.3416	2.1882	-.7019	.3220
		-14.0078	-2.4139	-2.0949	-1.9371	-1.9044
5	10.0	300.460	7.2361	3.2135	1.1970	.5842
		-21.7840	-19.8422	-19.5339	-19.3517	-19.2925
5	100.0	1391.7427	55.1929	24.7336	9.2683	.4534
		-195.2328	-193.2825	-192.9718	-192.7844	-192.7224

TABLE II  
UPSTREAM SINGULAR POINT EIGENVALUES  $\lambda_1$  and  $\lambda_2$

M $\alpha$	$\beta$				
	2	10	20	50	100
2 .001	1.8273 -0.9143	1.8420 -0.1764	1.8687 -0.8844	1.9581 -0.0352	2.1299 -0.0173
2 .02	1.8032 -0.9699	1.5586 -0.1899	1.4506 -0.0906	1.2428 -0.0306	1.0128 -0.0116
2 .10	1.7983 -0.1263	1.1774 -0.3868	.8628 -0.2600	.8798 -.2854	.4664 .0186
2 1.0	 	.2840 -2.1632	.0676 -0.1832	-0.0601 -0.0305	23.1508 -0.0488
2 10.0	 	1.5945 .7388	461.57 .1287	20.0975 -0.1846	6.9105 -0.1892
2 100.0	 	14.6016 16.8992	-2.3552 -1156.1	143.95 0.4270	-4.6616 -153.932

TABLE.II (contd)  
UPSTREAM SINGULAR POINT EIGENVALUES  $\lambda_1$  and  $\lambda_2$

M	$\alpha$	$\beta$				
		2	10	20	50	100
5	.001	2.4636 -1.0070	2.4845 -0.1868	2.5207 -0.0929	2.6416 -0.0366	2.8734 -0.0178
5	.02	2.4584 -1.0770	2.6119 -0.2045	3.1553 -0.0954	2.2185 -0.0287	2.2834 -0.6741
5	.10	2.5108 -1.4270	2.2318 -0.4015	2.5324 -0.2085	3.7770 -0.0602	.4528 -0.0262
5	1.0		835.934 1.0283	84.4784 .7390	19.3834 0.4722	14.111 .2600
5	10.0		9521.9	892.34	183.658	11.4059
5	100.0		95719.9	8872.88	1797.53	1028.26
			72.875	52.047	26.612	53.948

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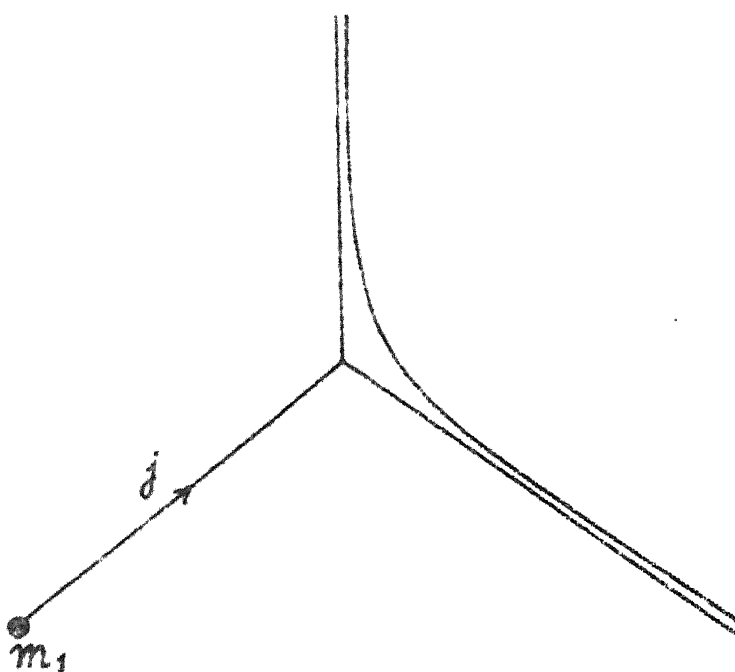


Fig 1(a) Trajectory of molecule  $m_2$  relative to molecule  $m_1$

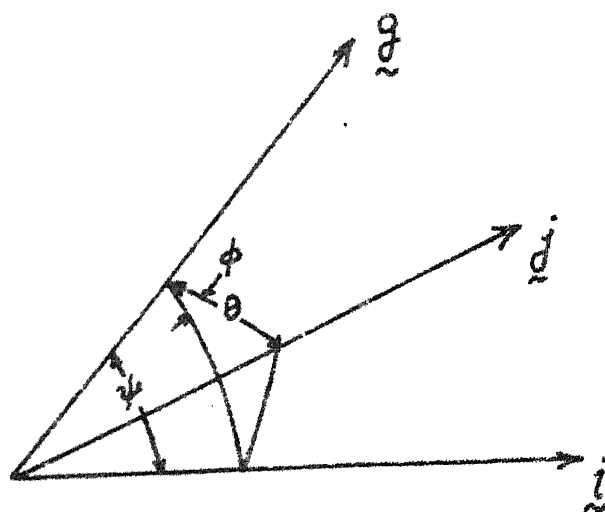


Fig 1(b) Orientation ( in space ) of vectors  $\underline{i}$  ,  $\underline{j}$  ,  $\underline{g}$

Phase-Plane Diagram

$$\alpha = 0.1$$

$$\beta = 10.0$$

$$M = 2.0$$

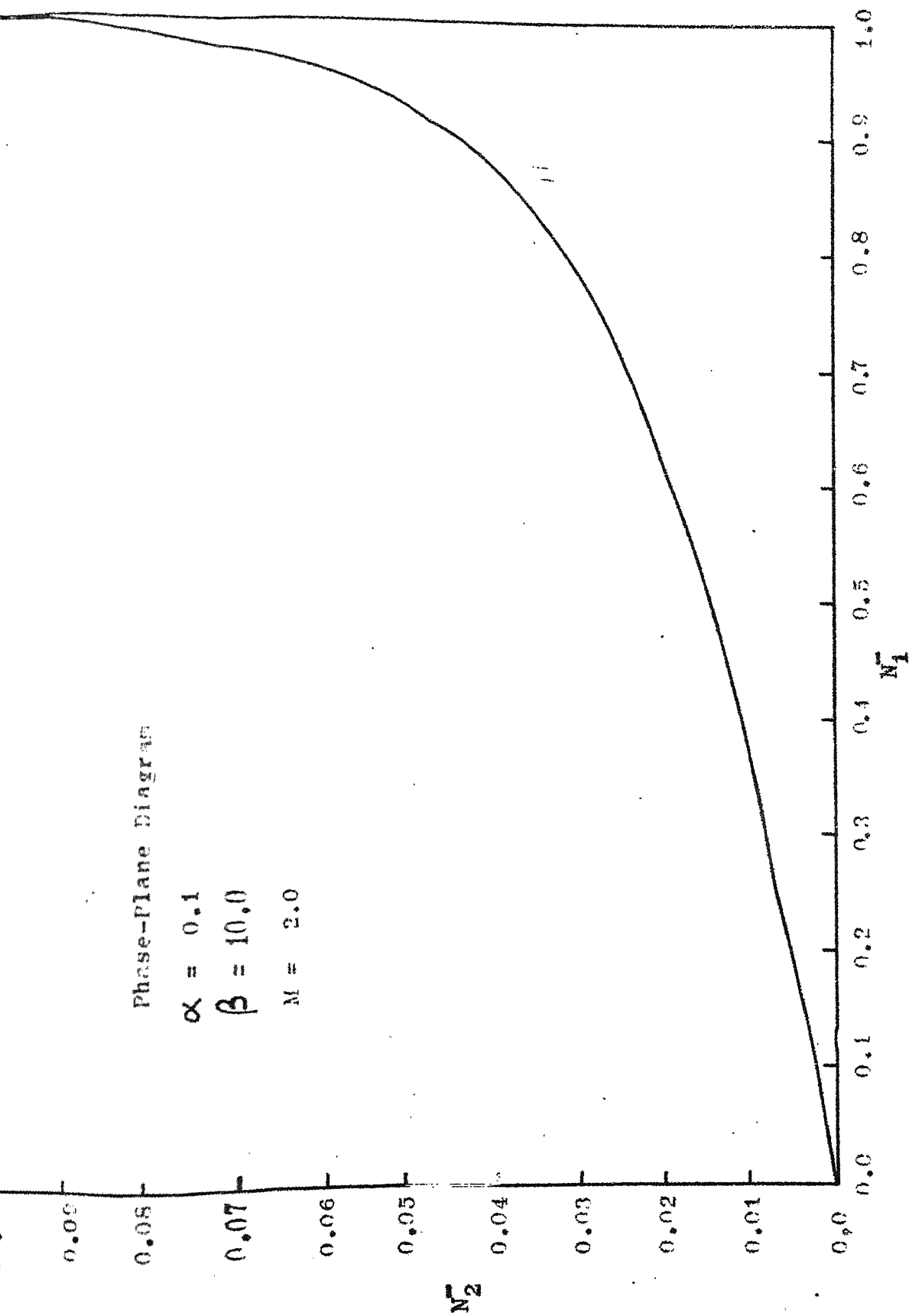


FIG. 2 PHASE PLANE DIAGRAM

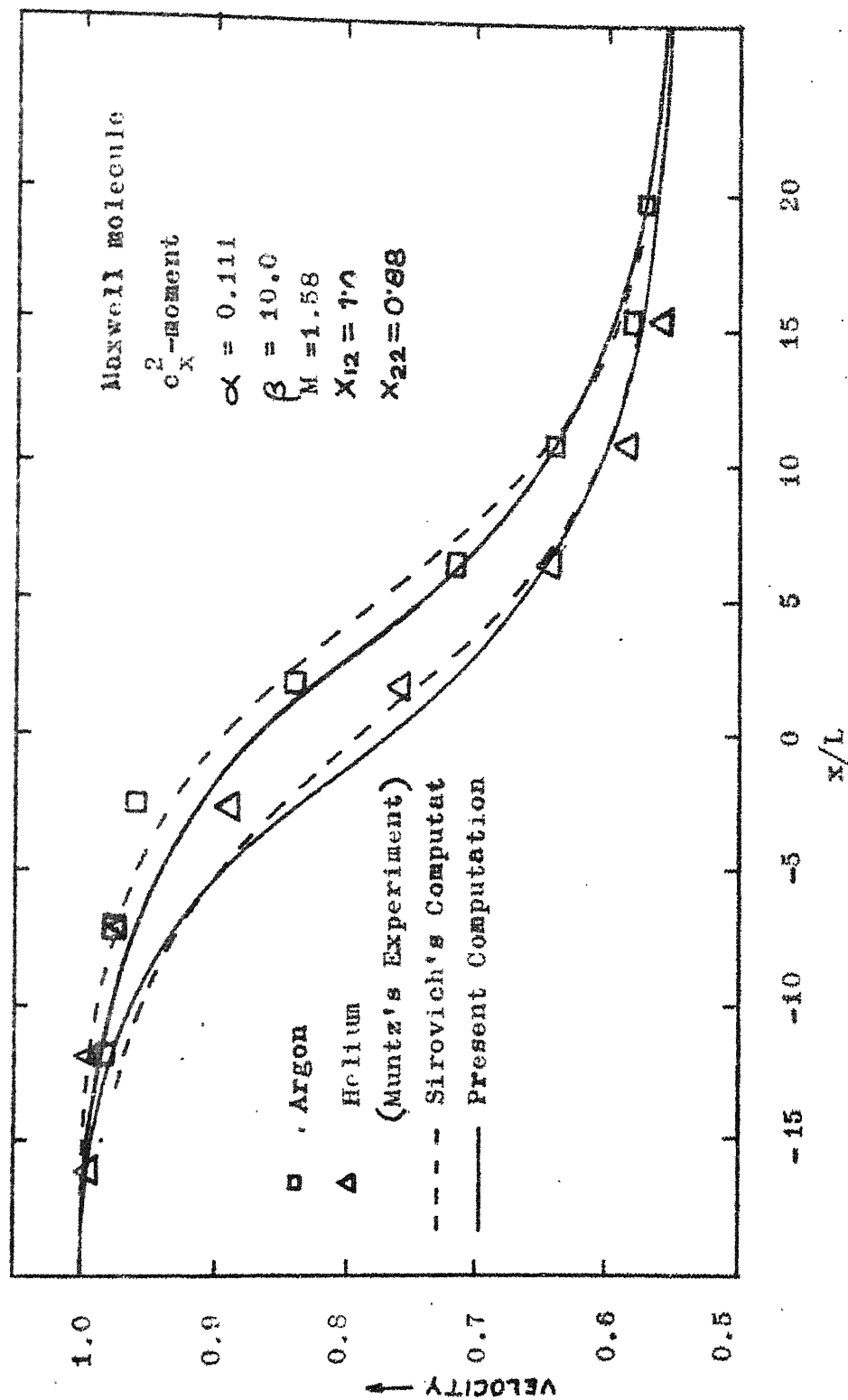


FIG3 VELOCITY PROFILE-COMPARISON WITH EXPERIMENT

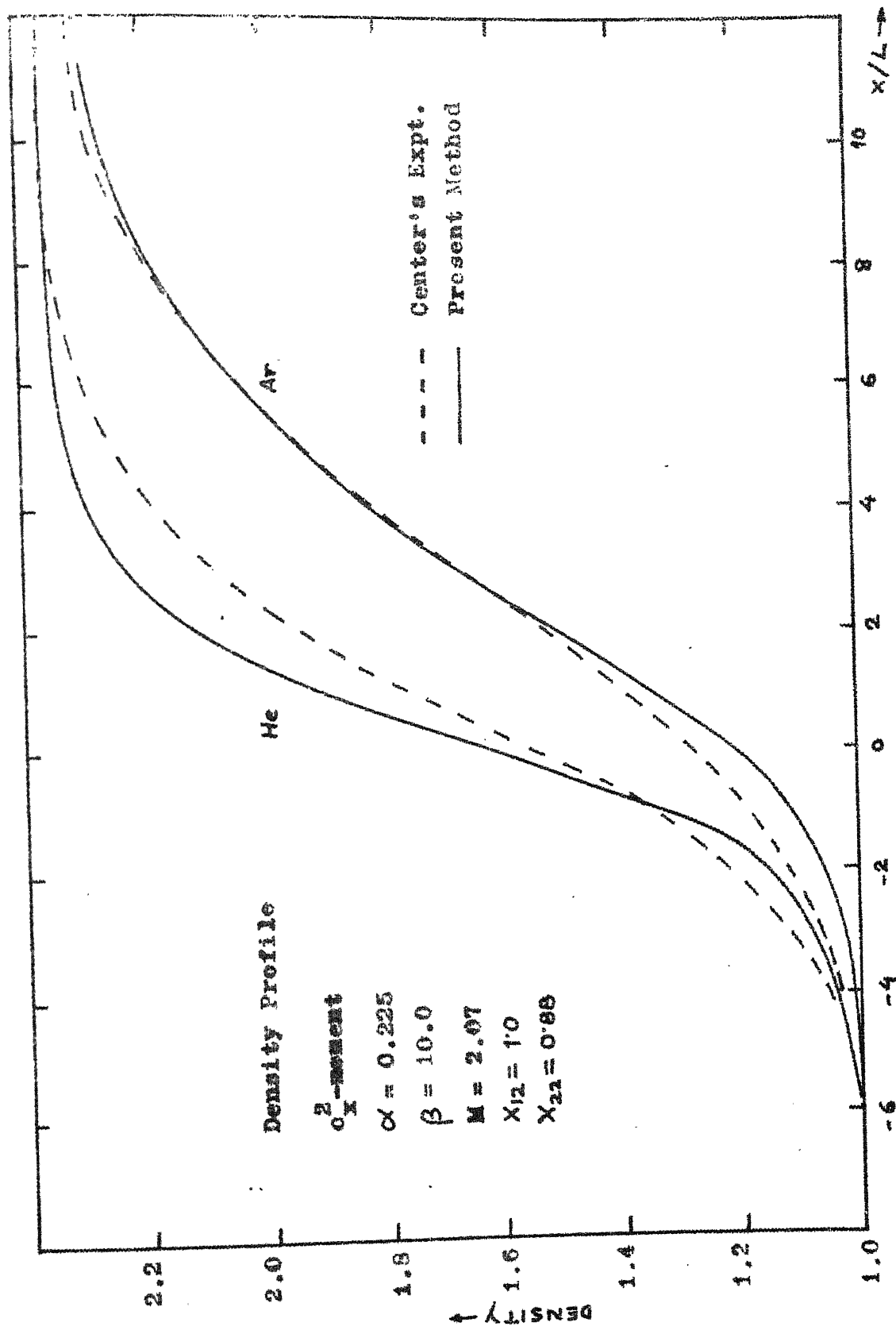
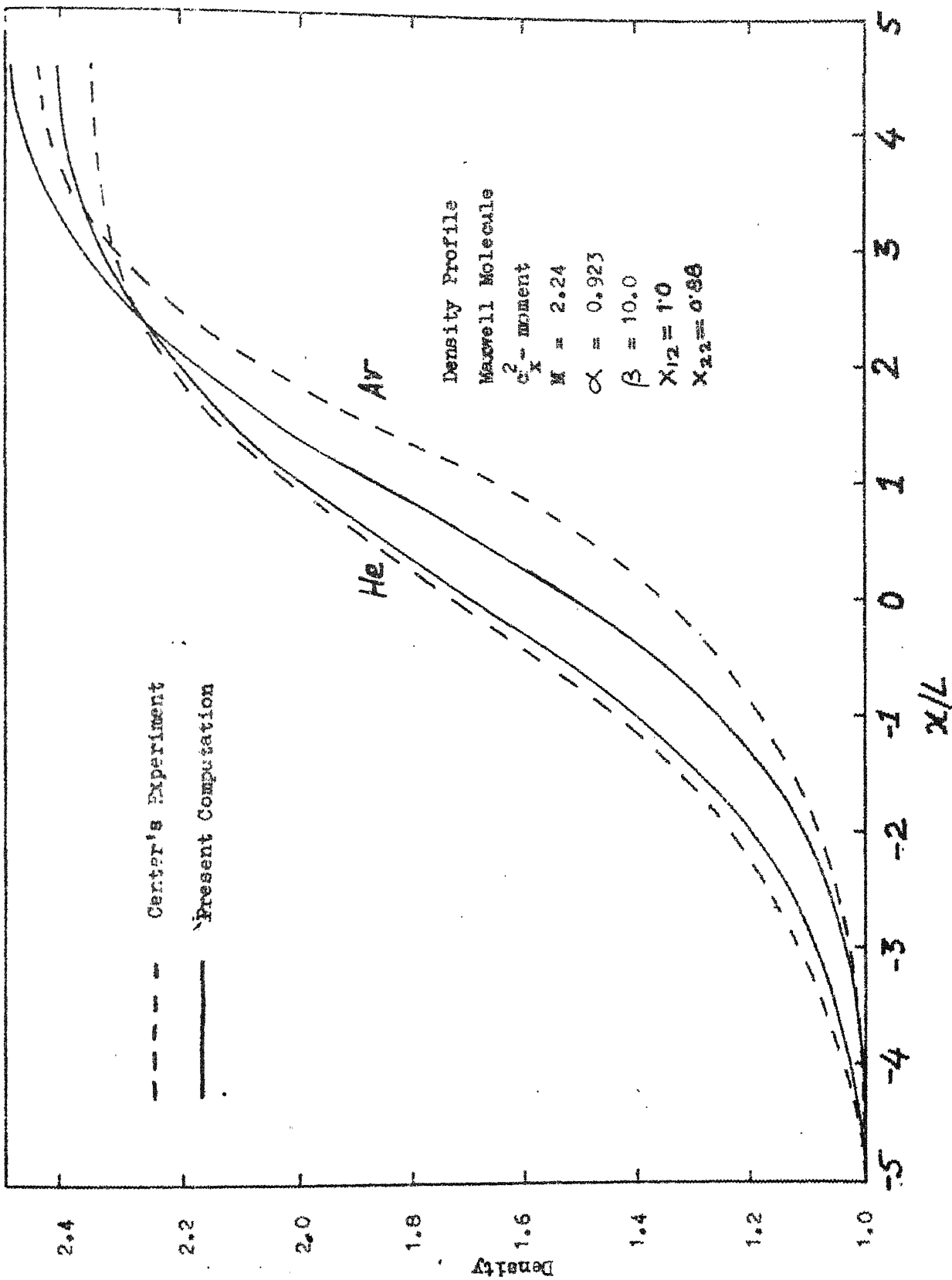


FIG 4 DENSITY PROFILE - COMPARISON WITH EXPERIMENT



FIGS DENSITY PROFILE - COMPARISON WITH EXPERIMENT

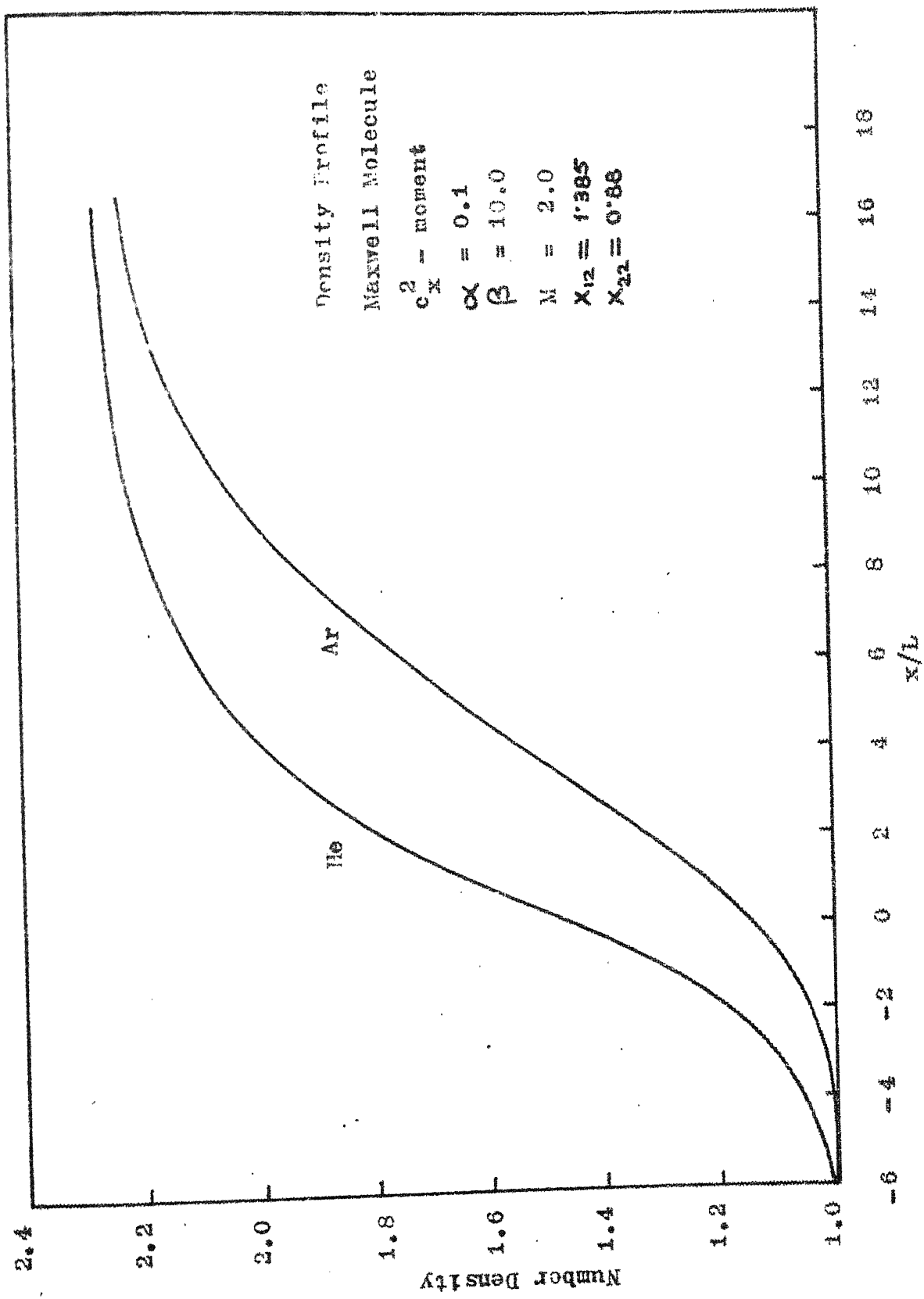


FIG 6 DENSITY PROFILE



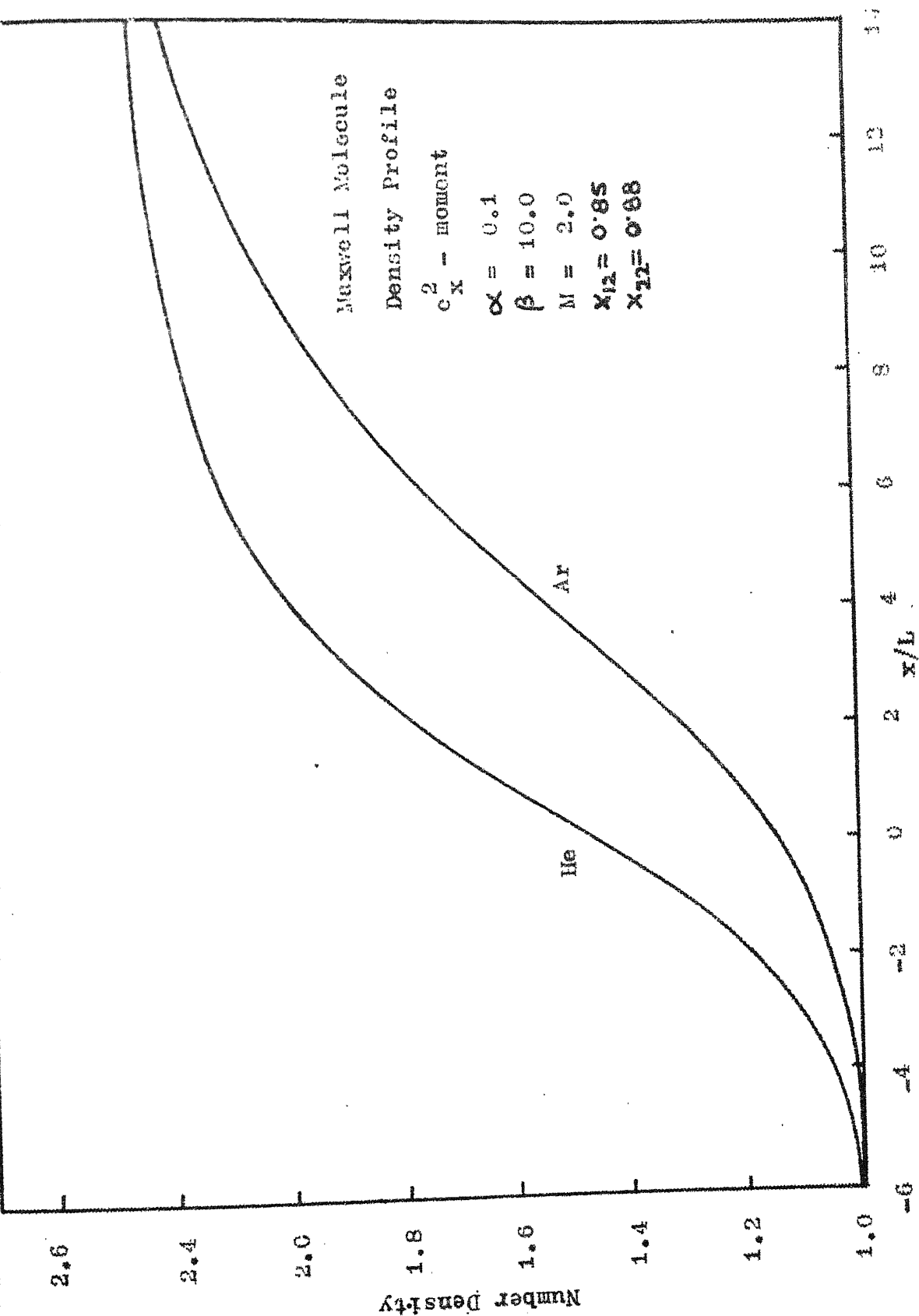


FIG 7 DENSITY PROFILE

# 8<sup>th</sup> ORDER RUNGE-KUTTA INTEGRATION

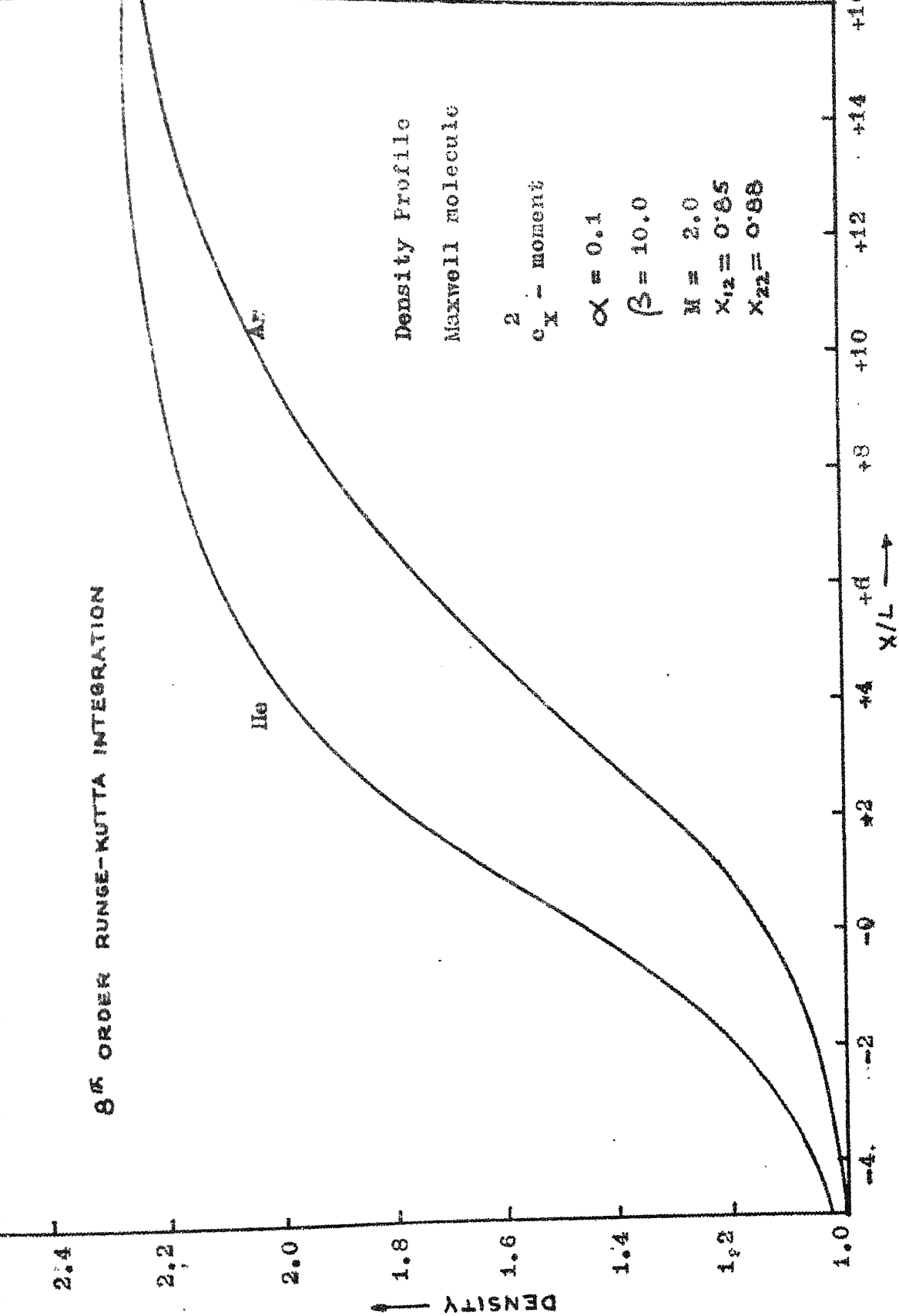


FIG 8 DENSITY PROFILE

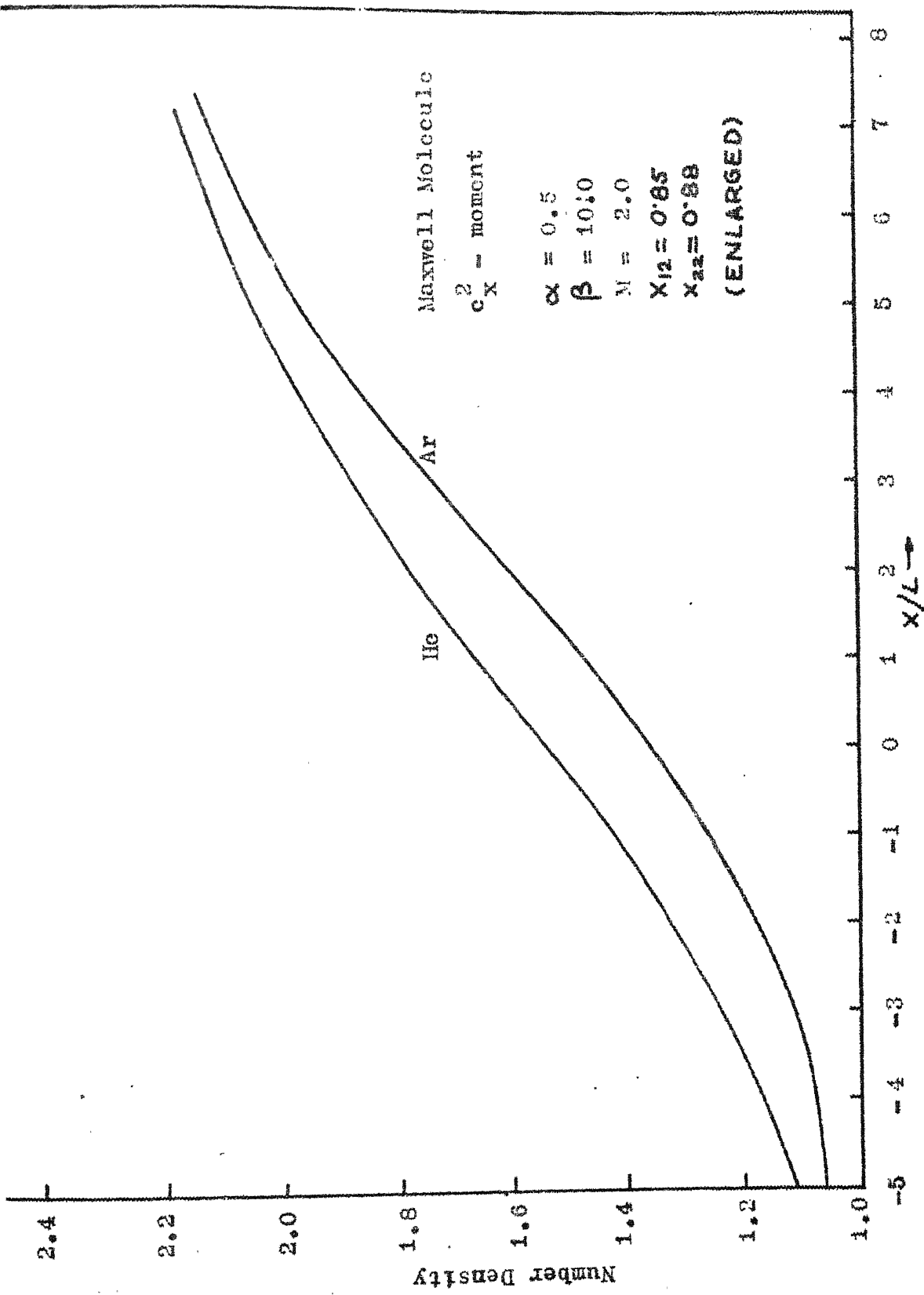


FIG 9 DENSITY PROFILE

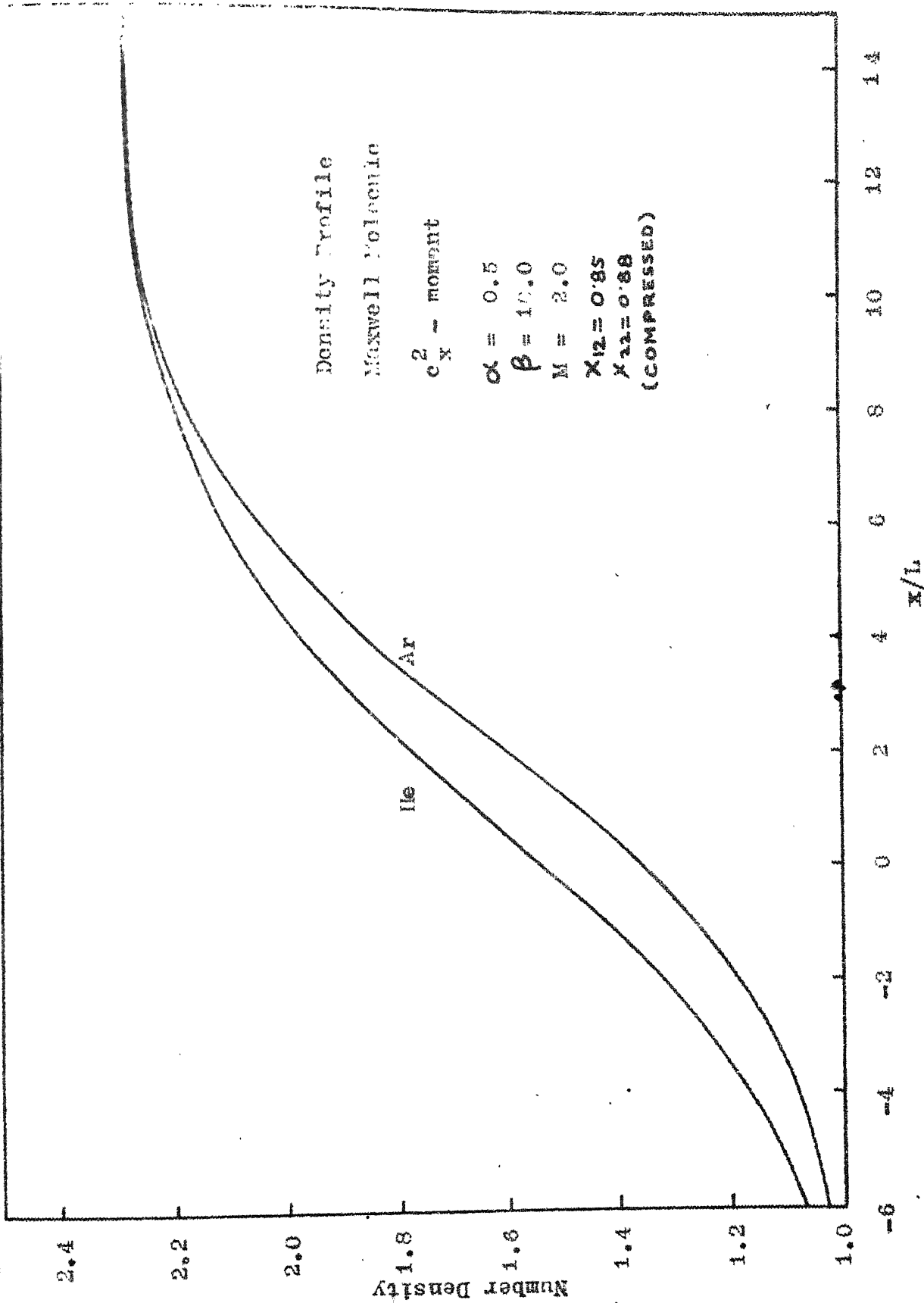


FIG 10 DENSITY PROFILE

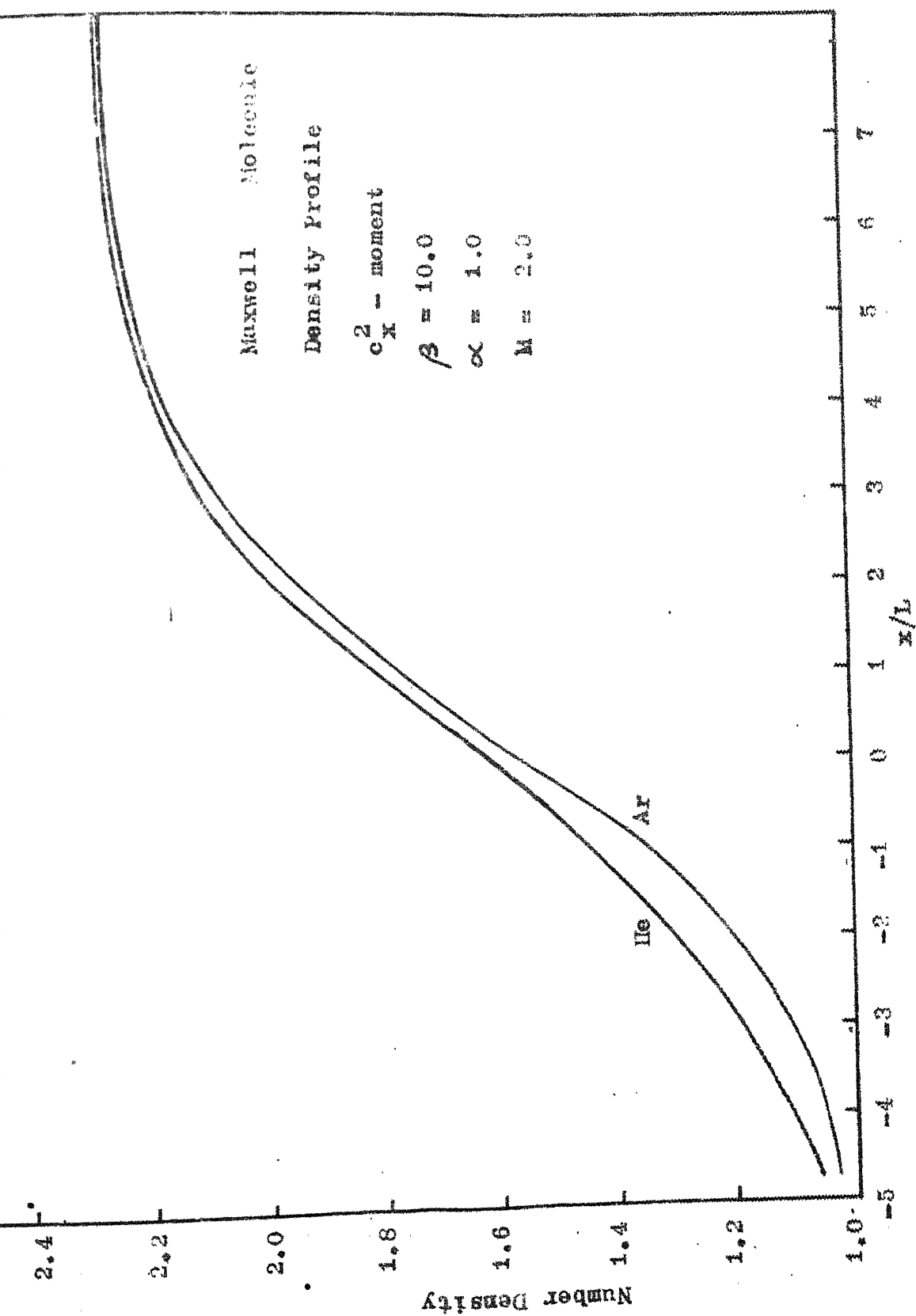


FIG 11 DENSITY PROFILE

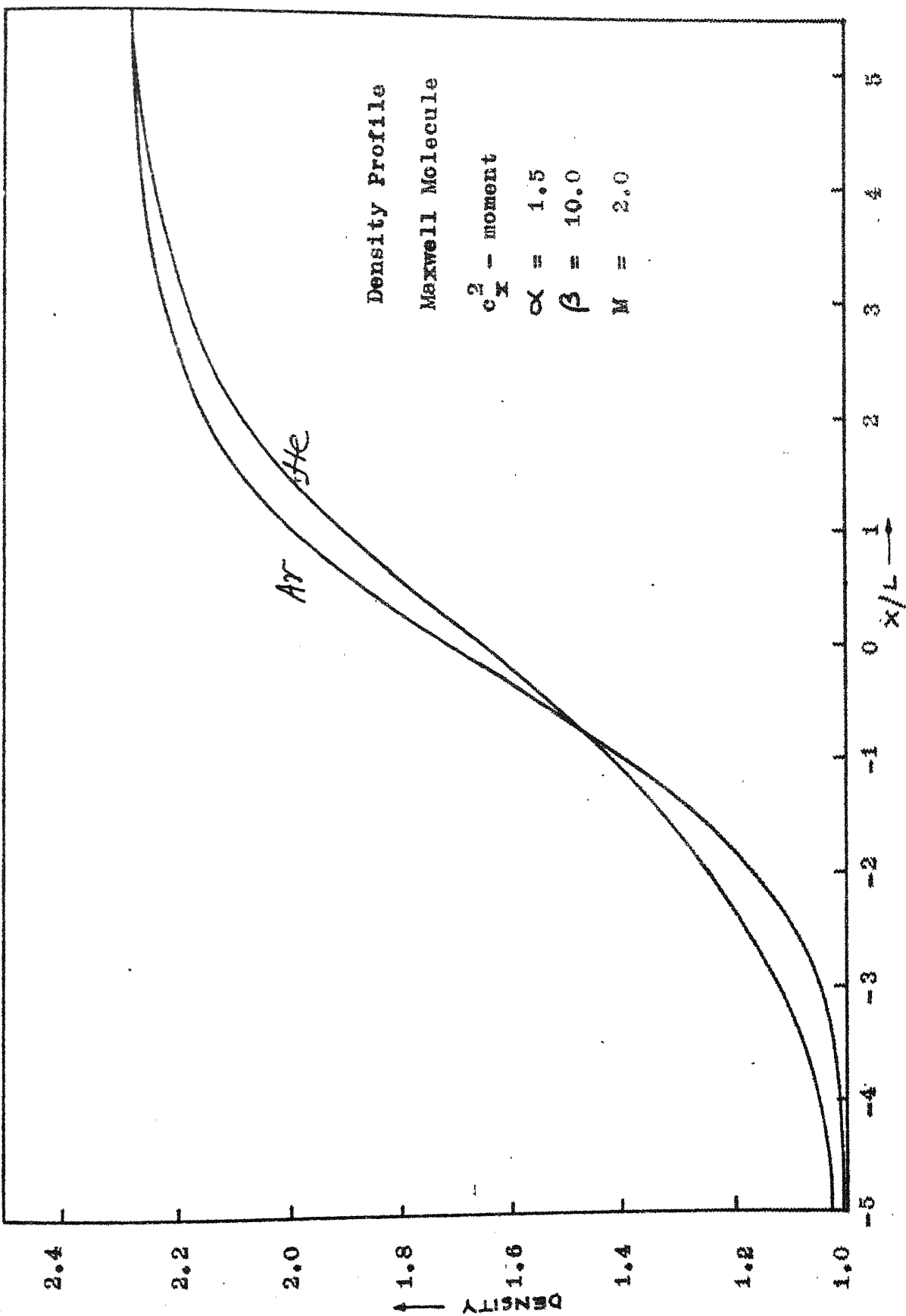


FIG 12 DENSITY PROFILE

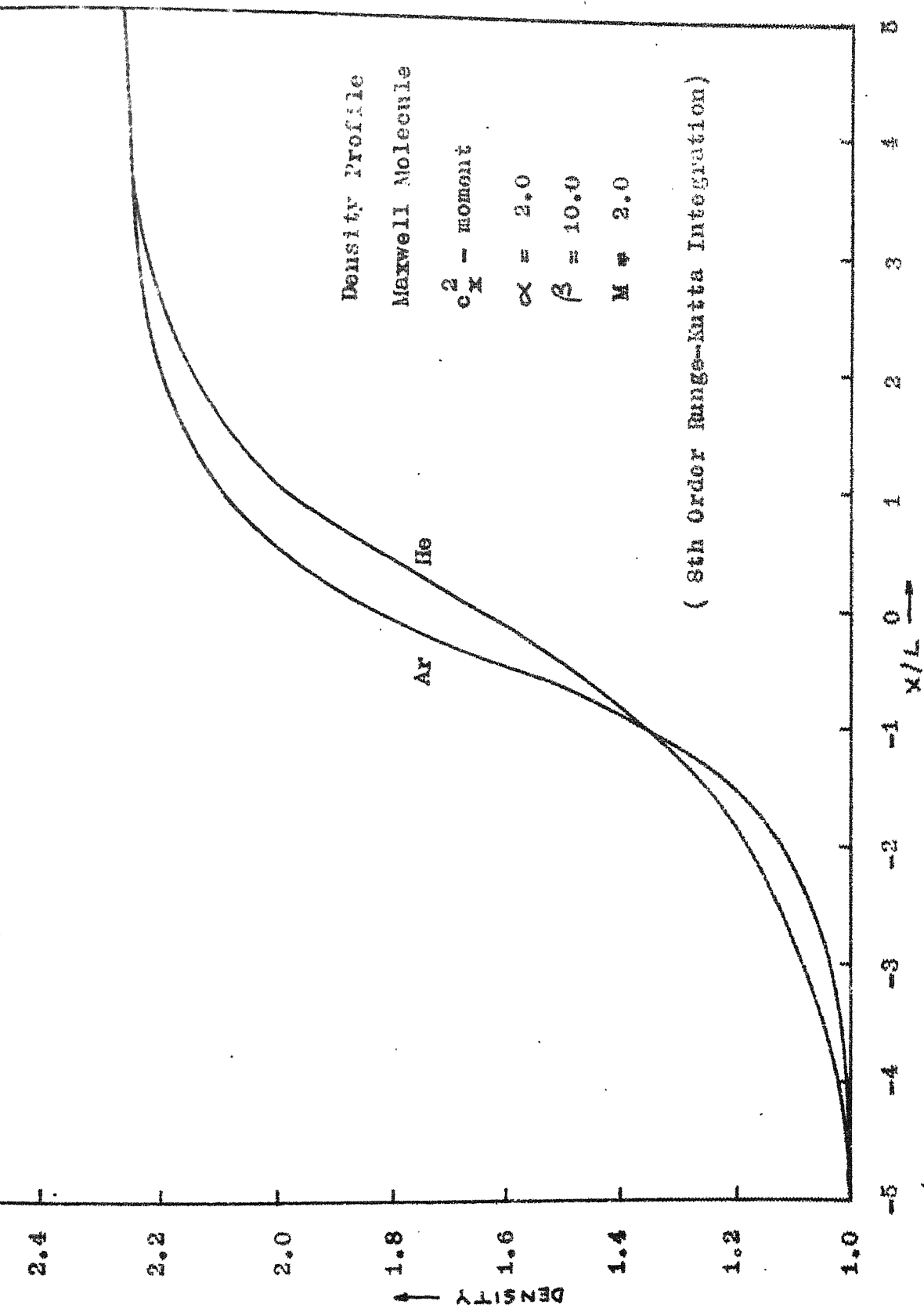


FIG 13 DENSITY PROFILE

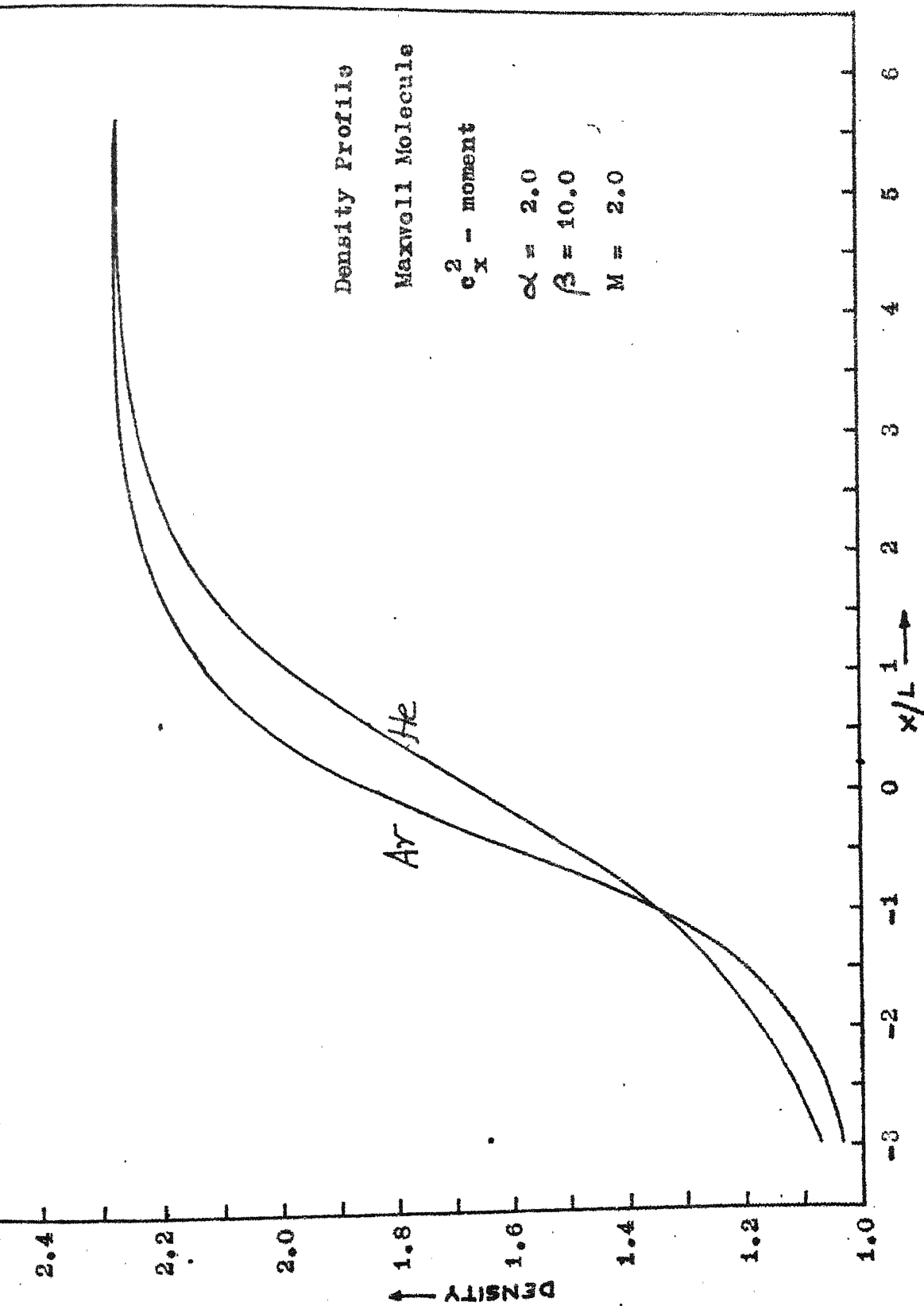


FIG 14 DENSITY PROFILE



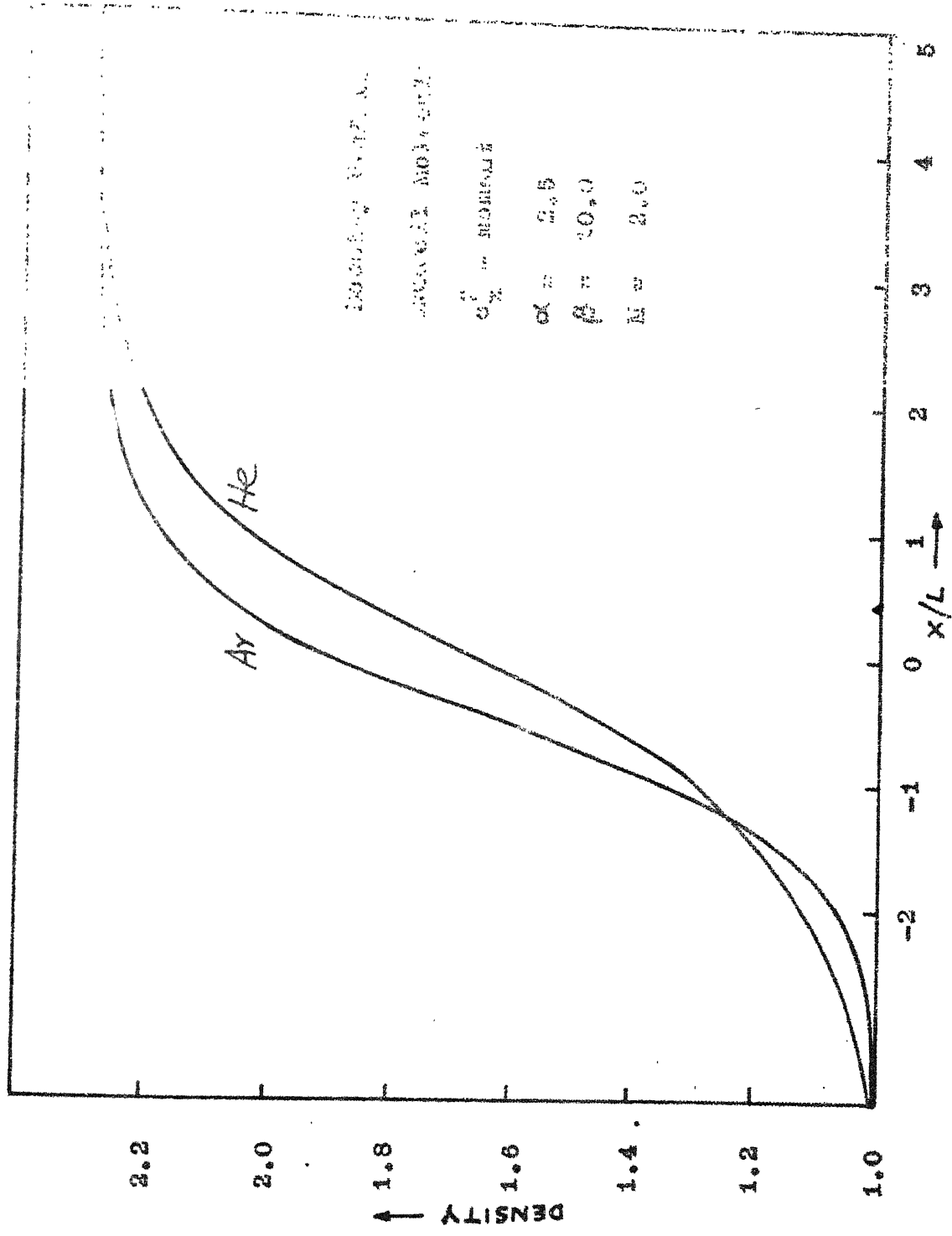


FIG 15 DENSITY PROFILE

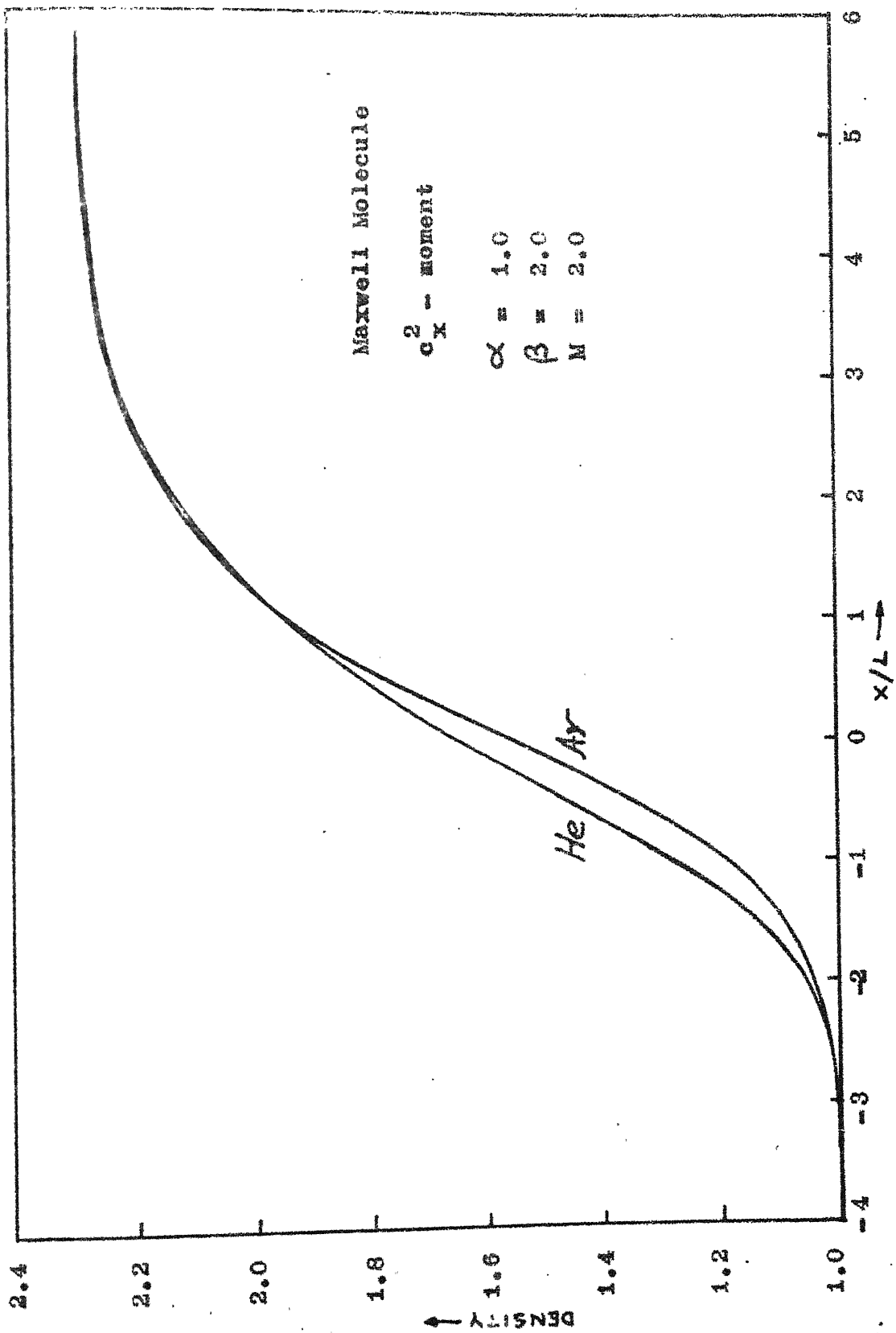


FIG 17 DENSITY PROFILE

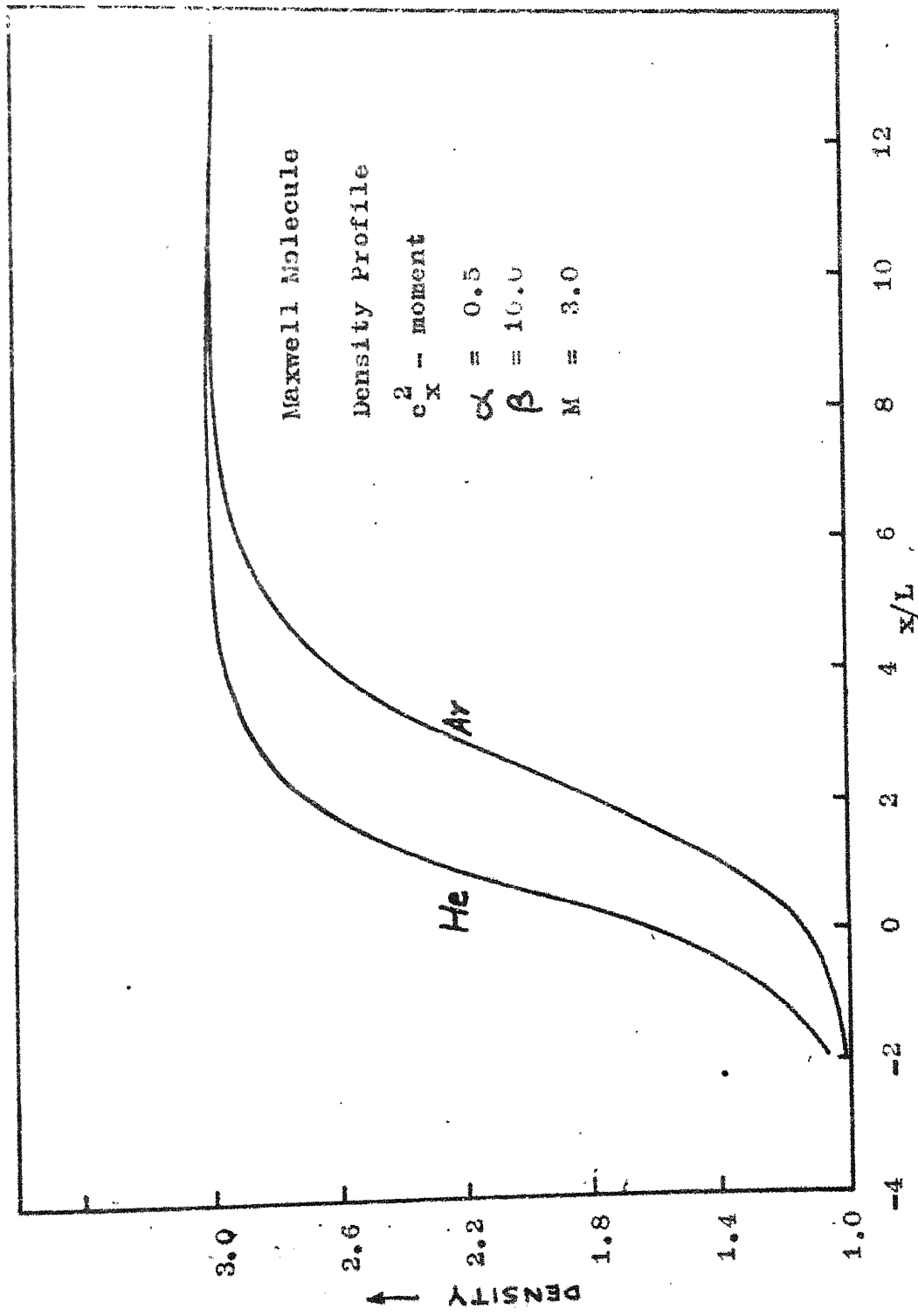


FIG 18 DENSITY PROFILE

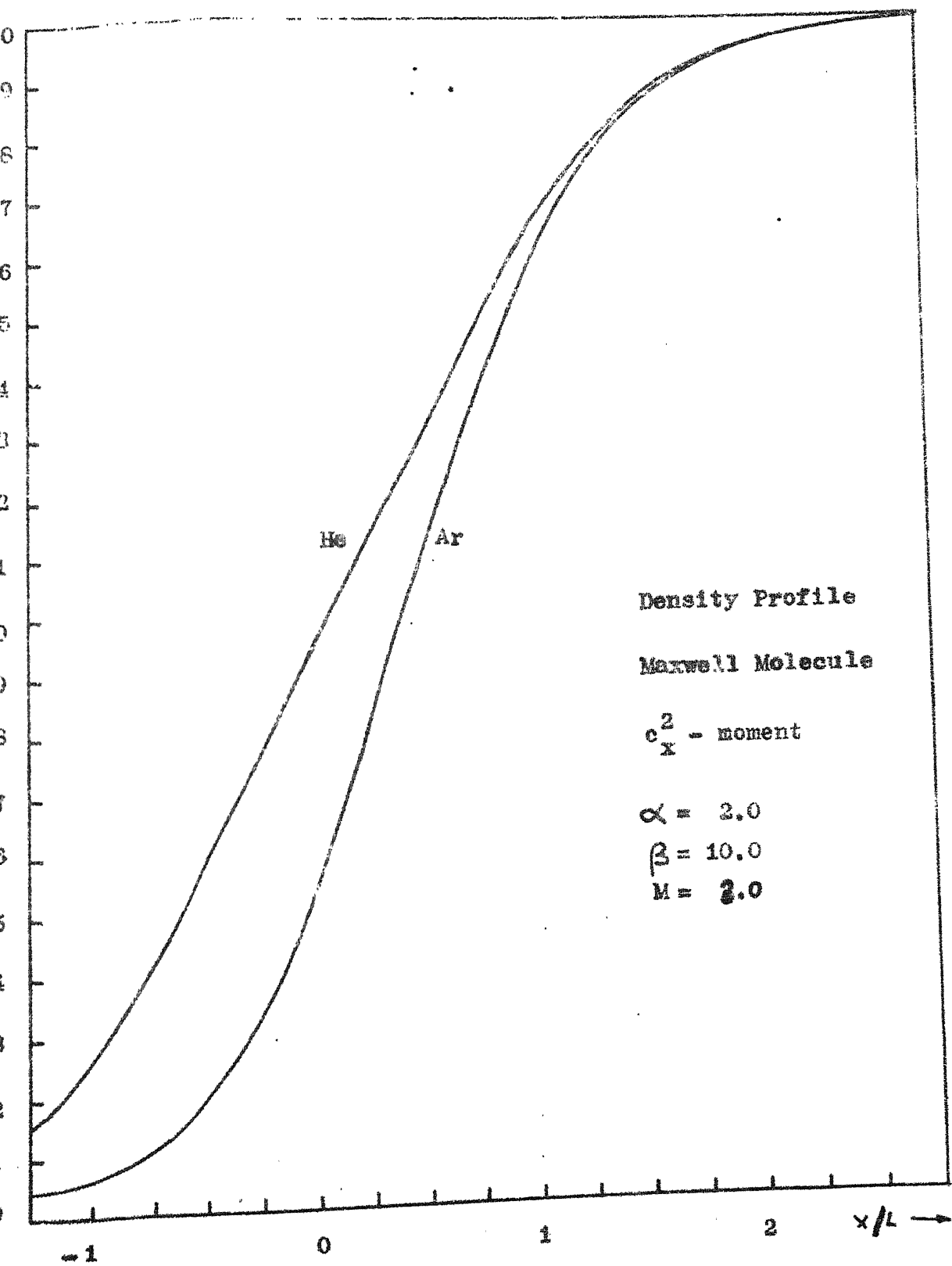


FIG 19 DENSITY PROFILE

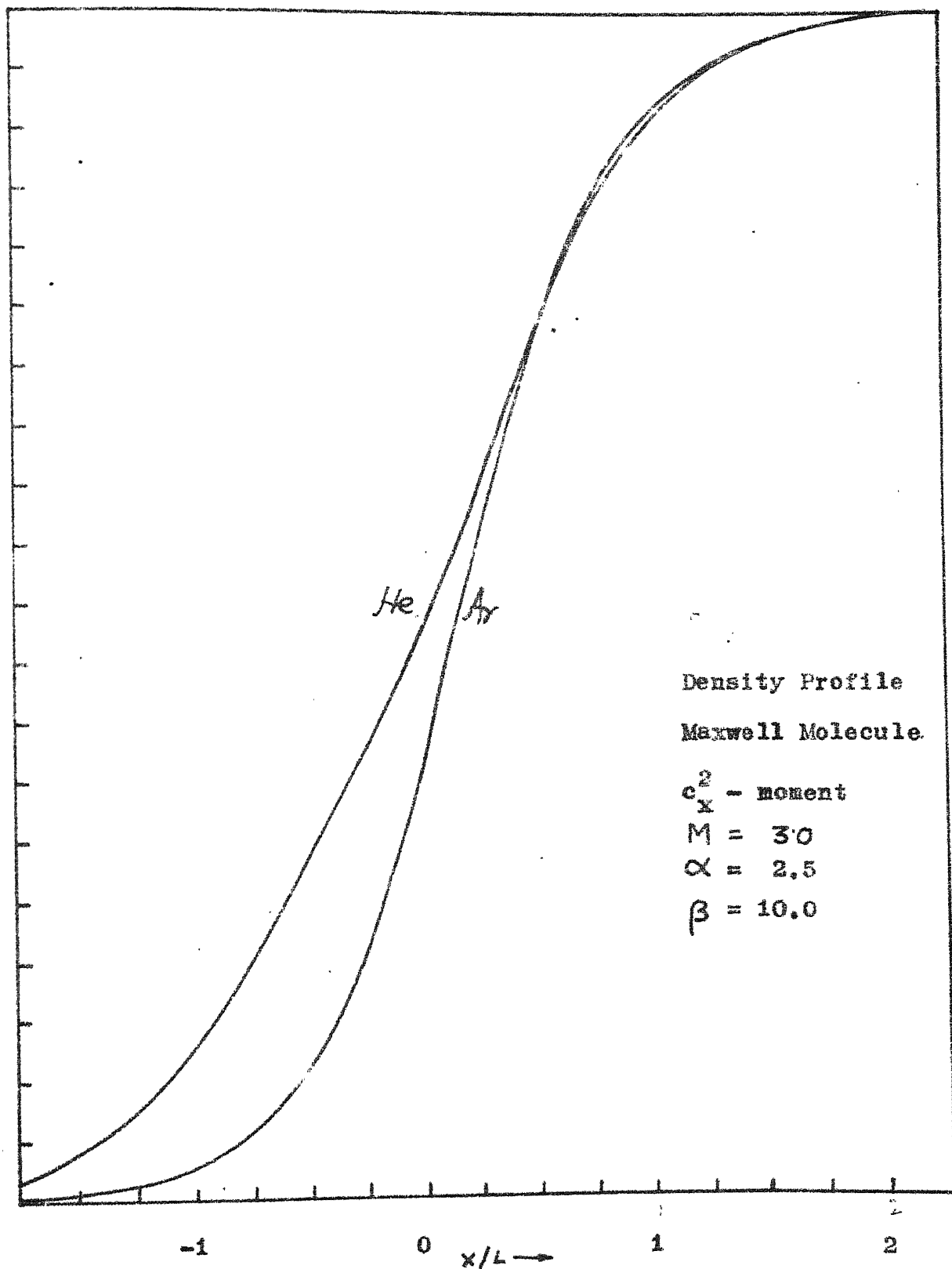


FIG 20 DENSITY PROFILE

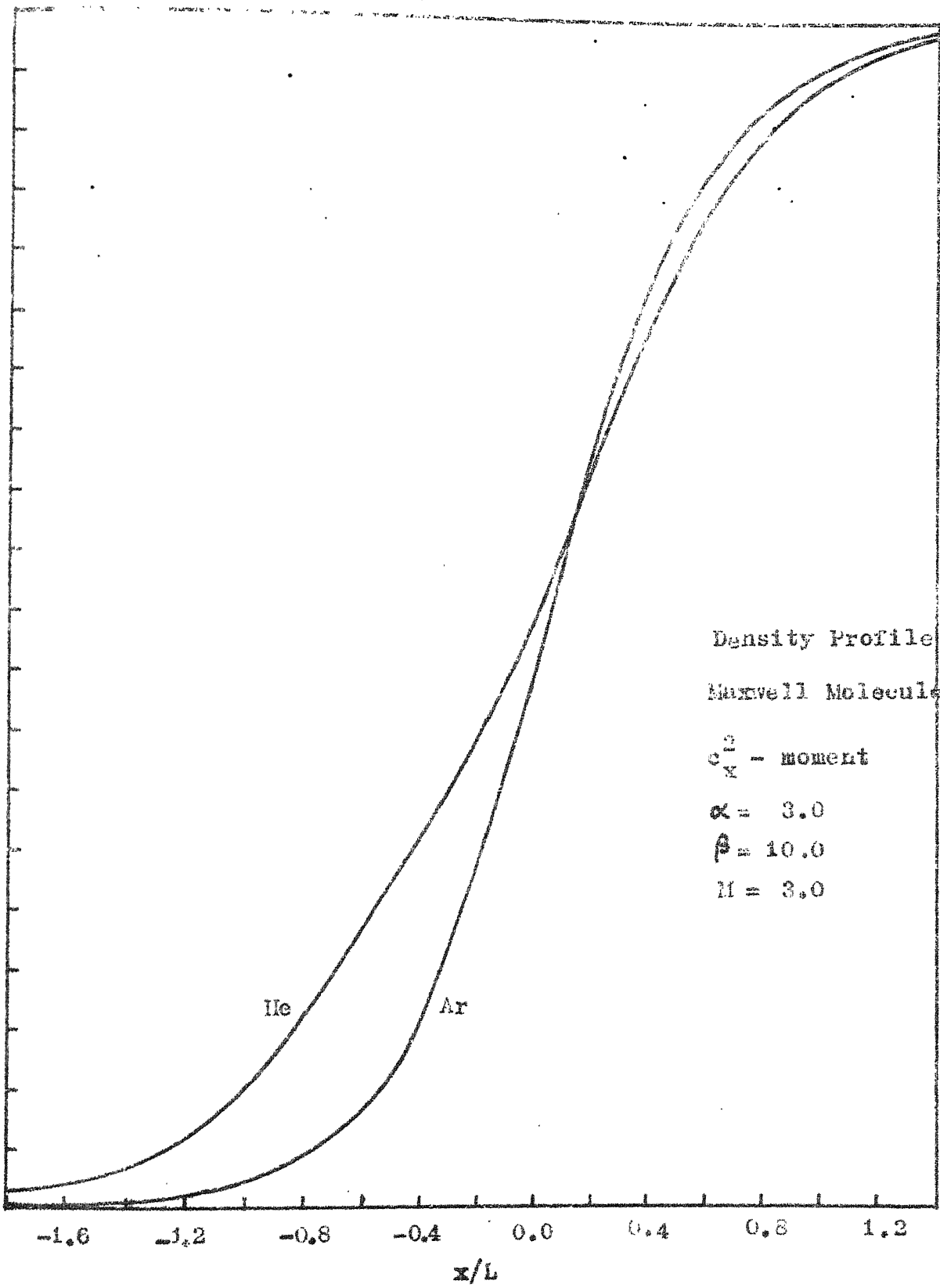


FIG 21 DENSITY PROFILE

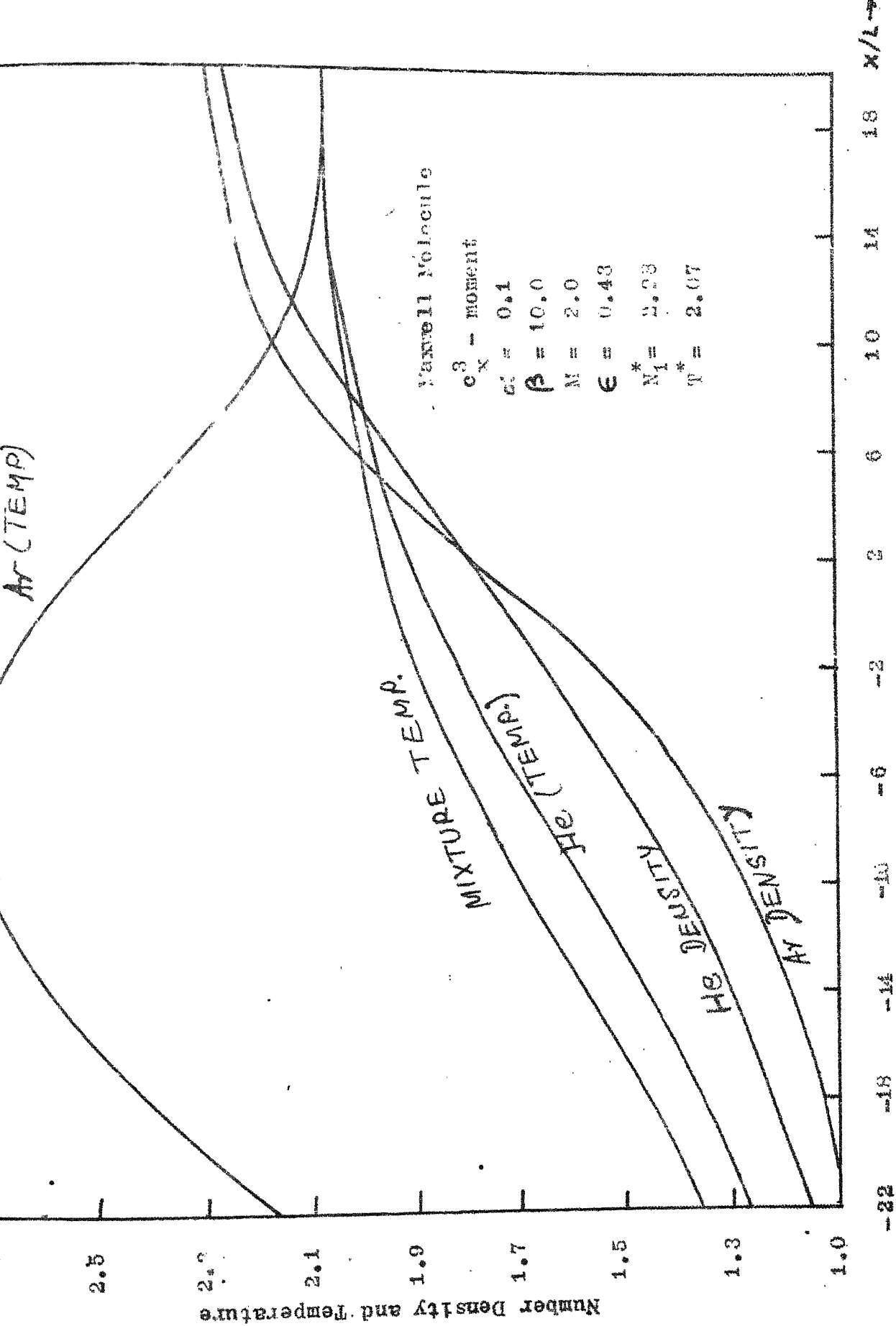


FIG 22 TEMPERATURE AND DENSITY PROFILES

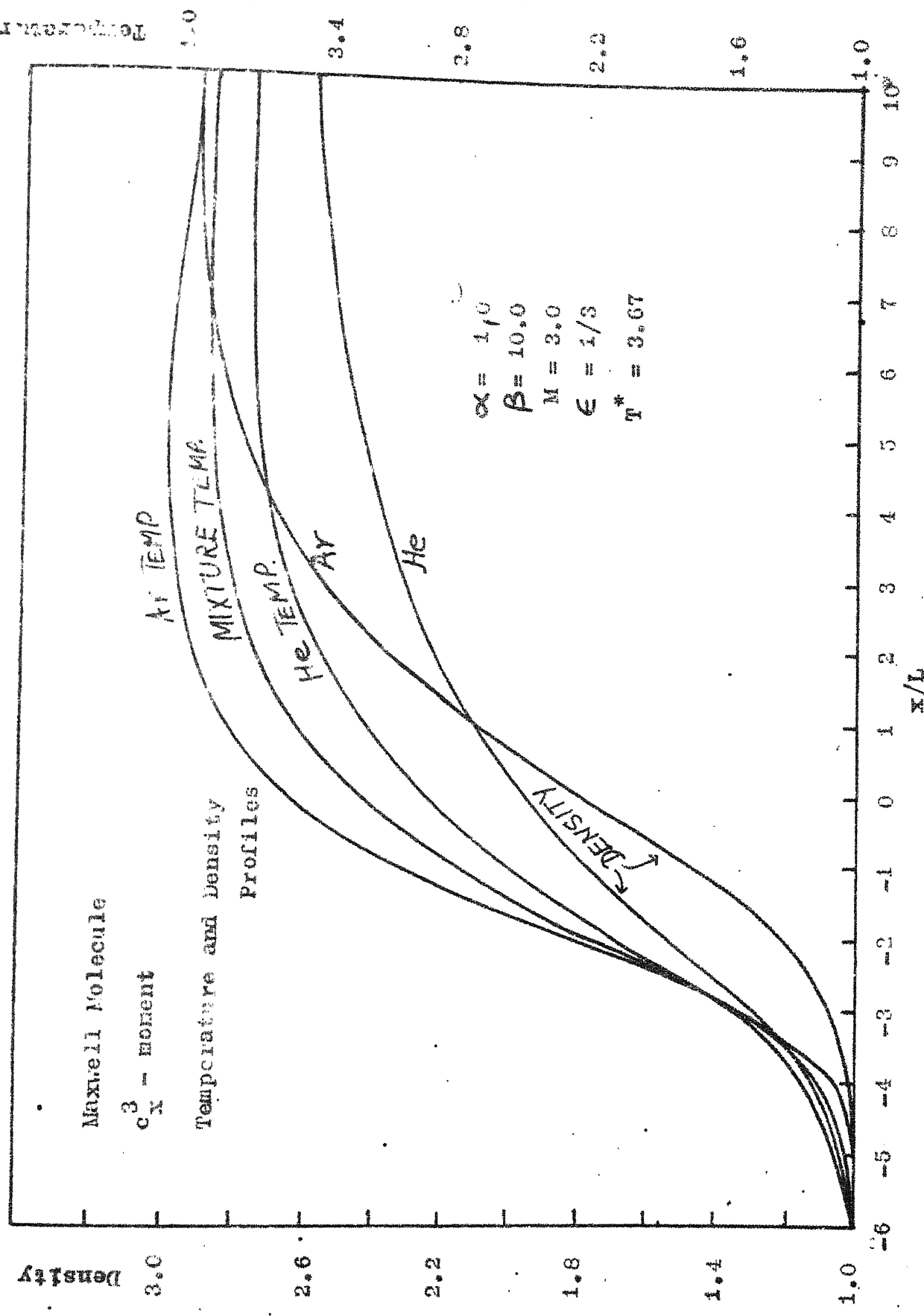


FIG 23 TEMPERATURE AND DENSITY PROFILES



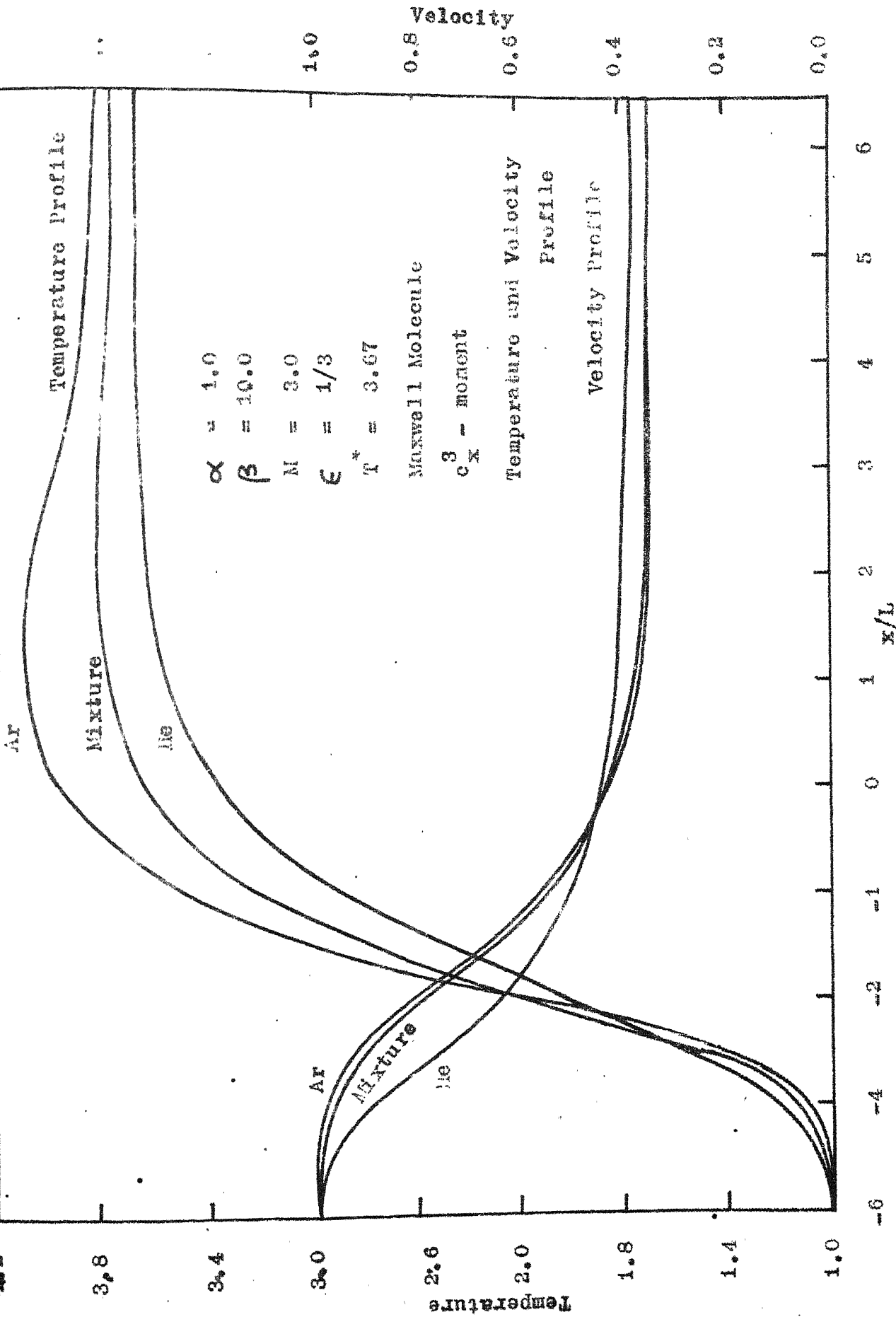


FIG 24 TEMPERATURE AND VELOCITY PROFILE

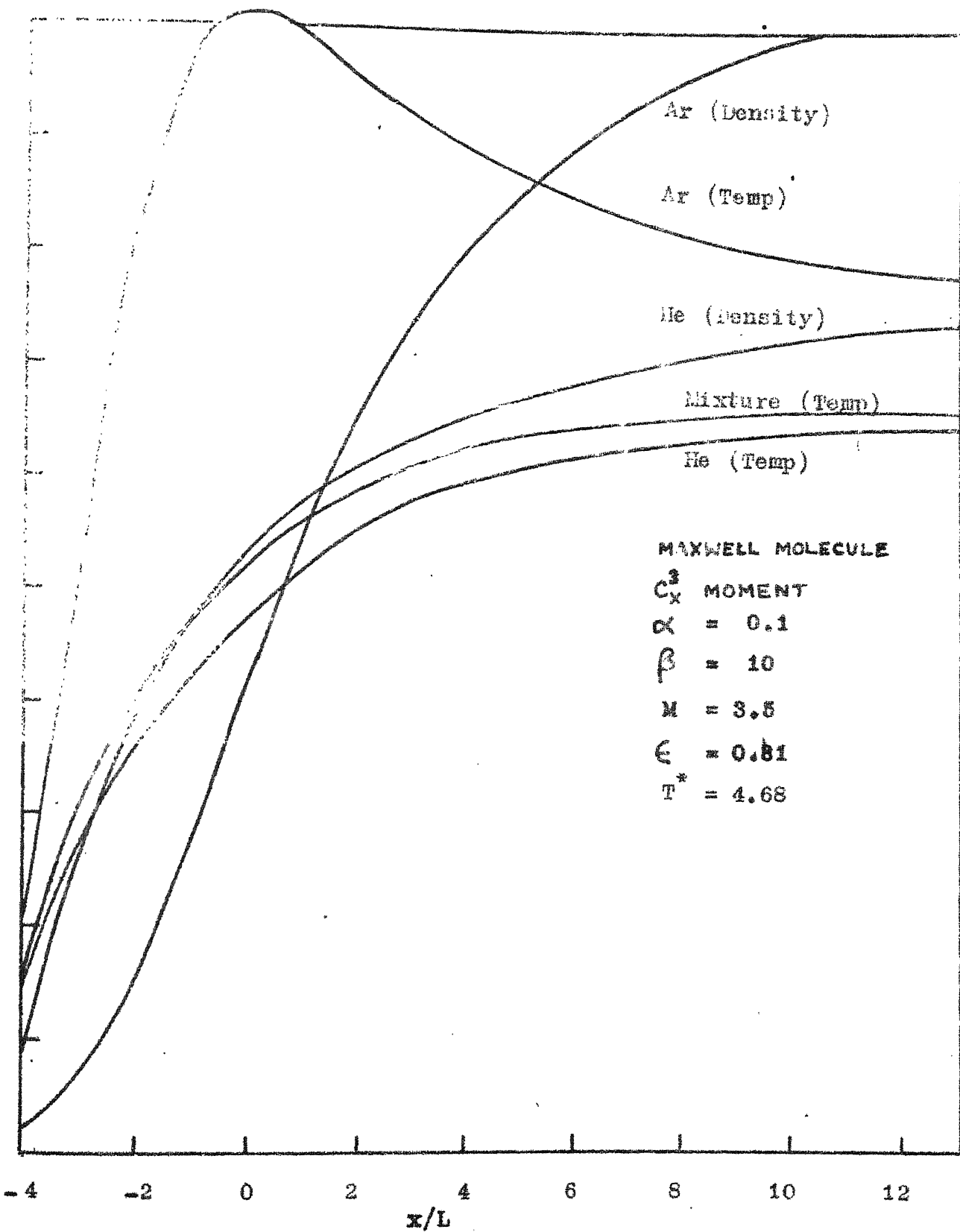


FIG 25 TEMPERATURE AND DENSITY PROFILES

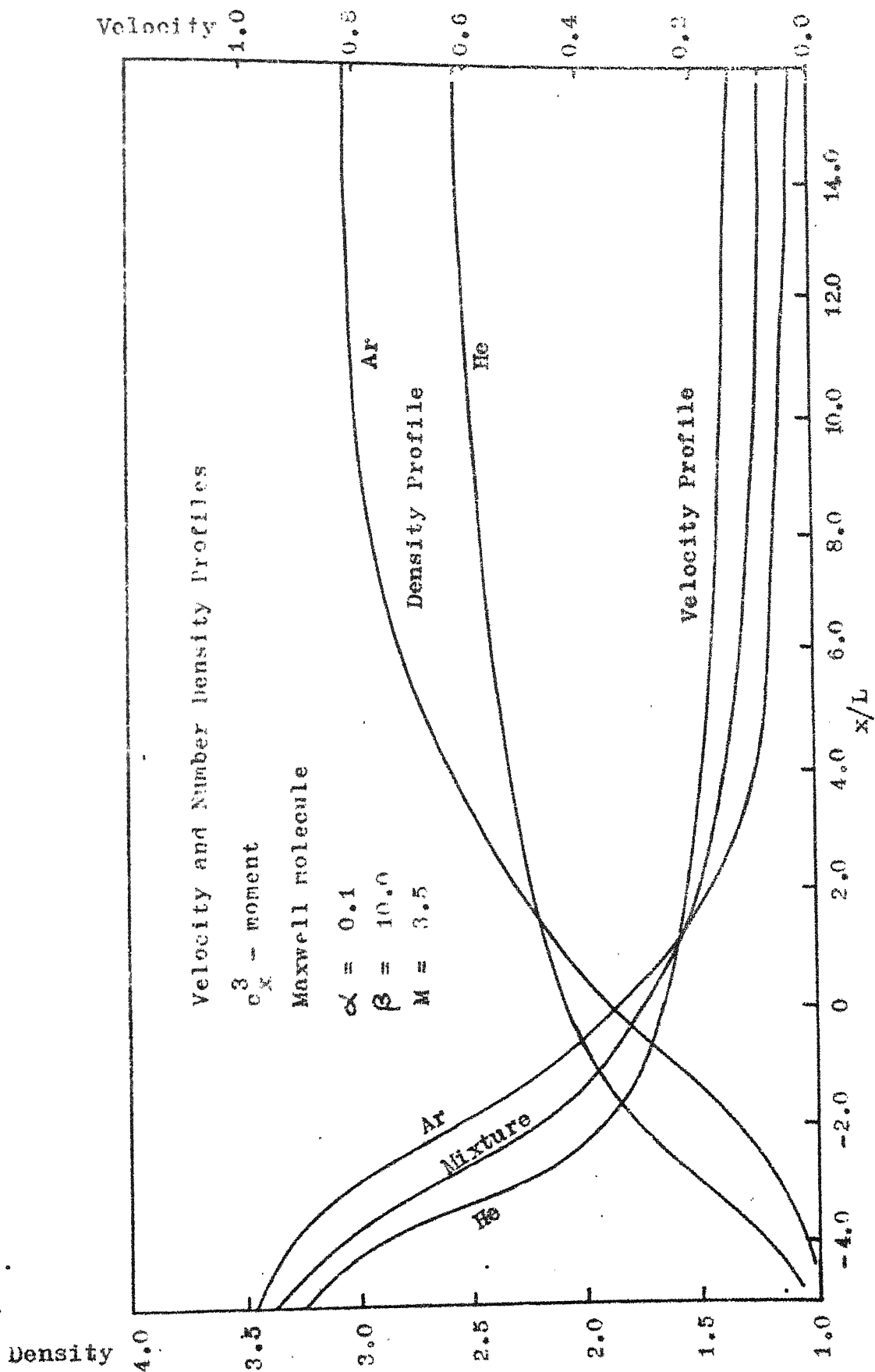


FIG 26 VELOCITY AND DENSITY PROFILE

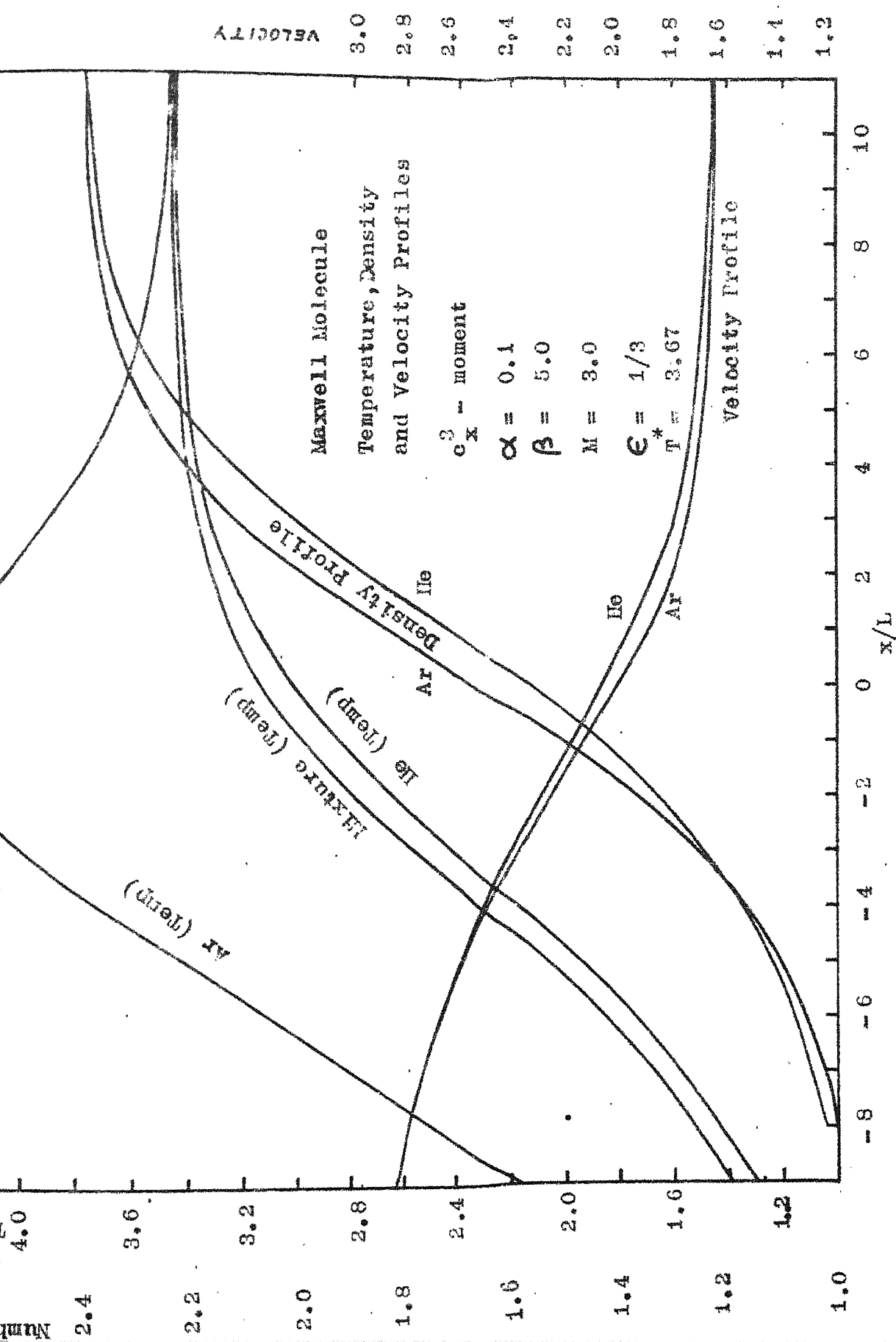


FIG 27 TEMPERATURE, DENSITY AND VELOCITY PROFILE

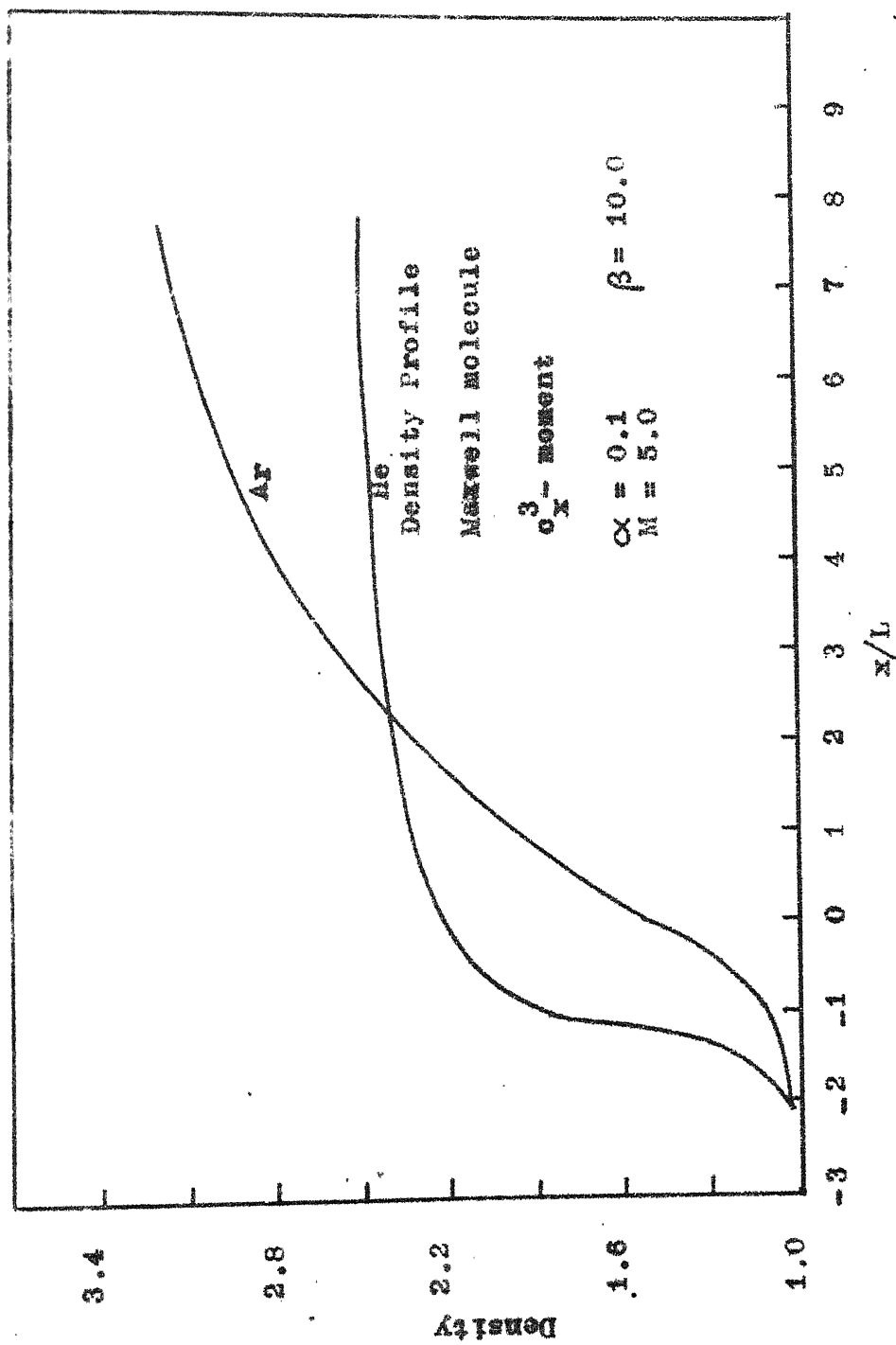


FIG 28 DENSITY PROFILE

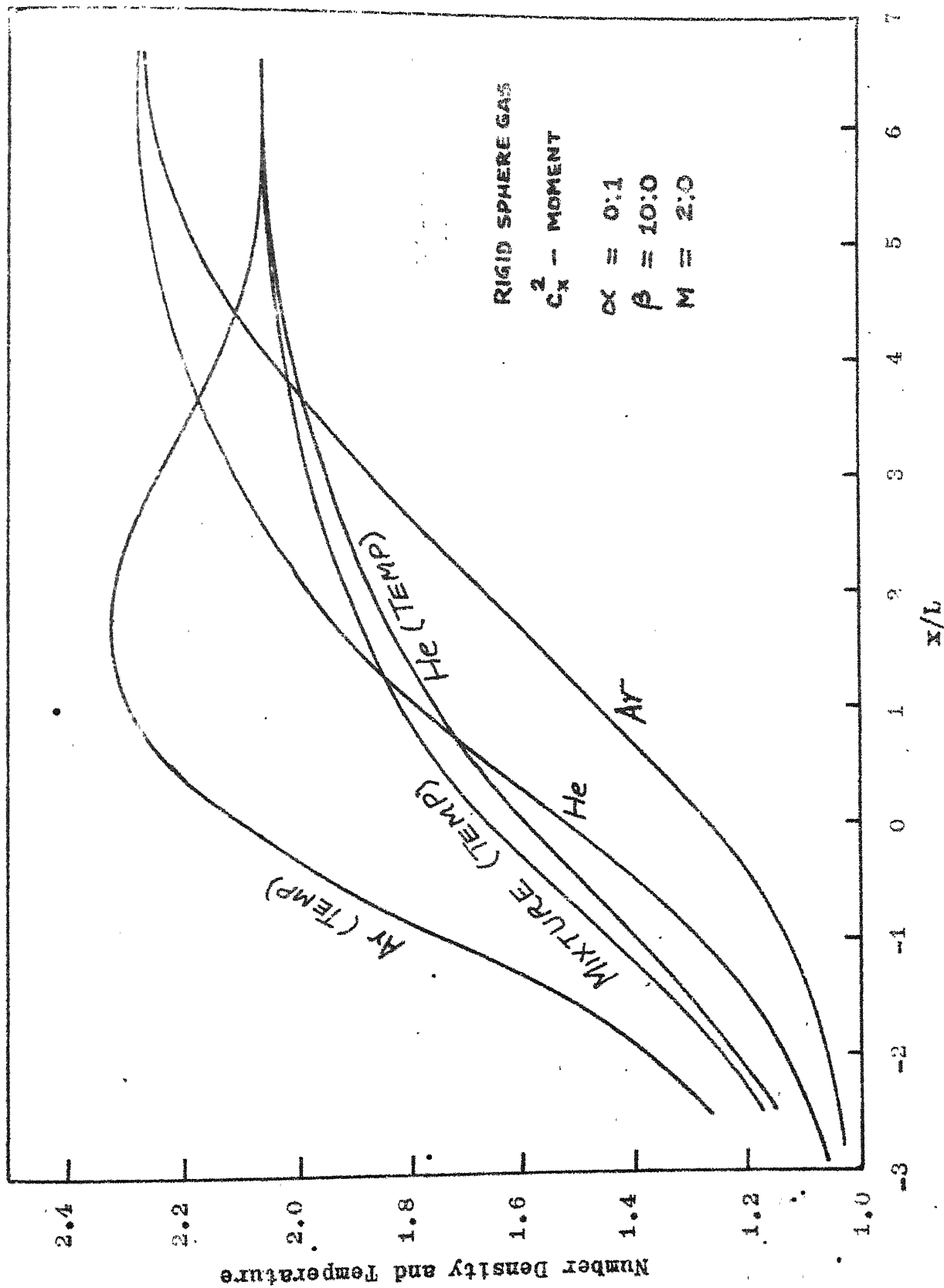


FIG 29 TEMPERATURE AND DENSITY PROFILES

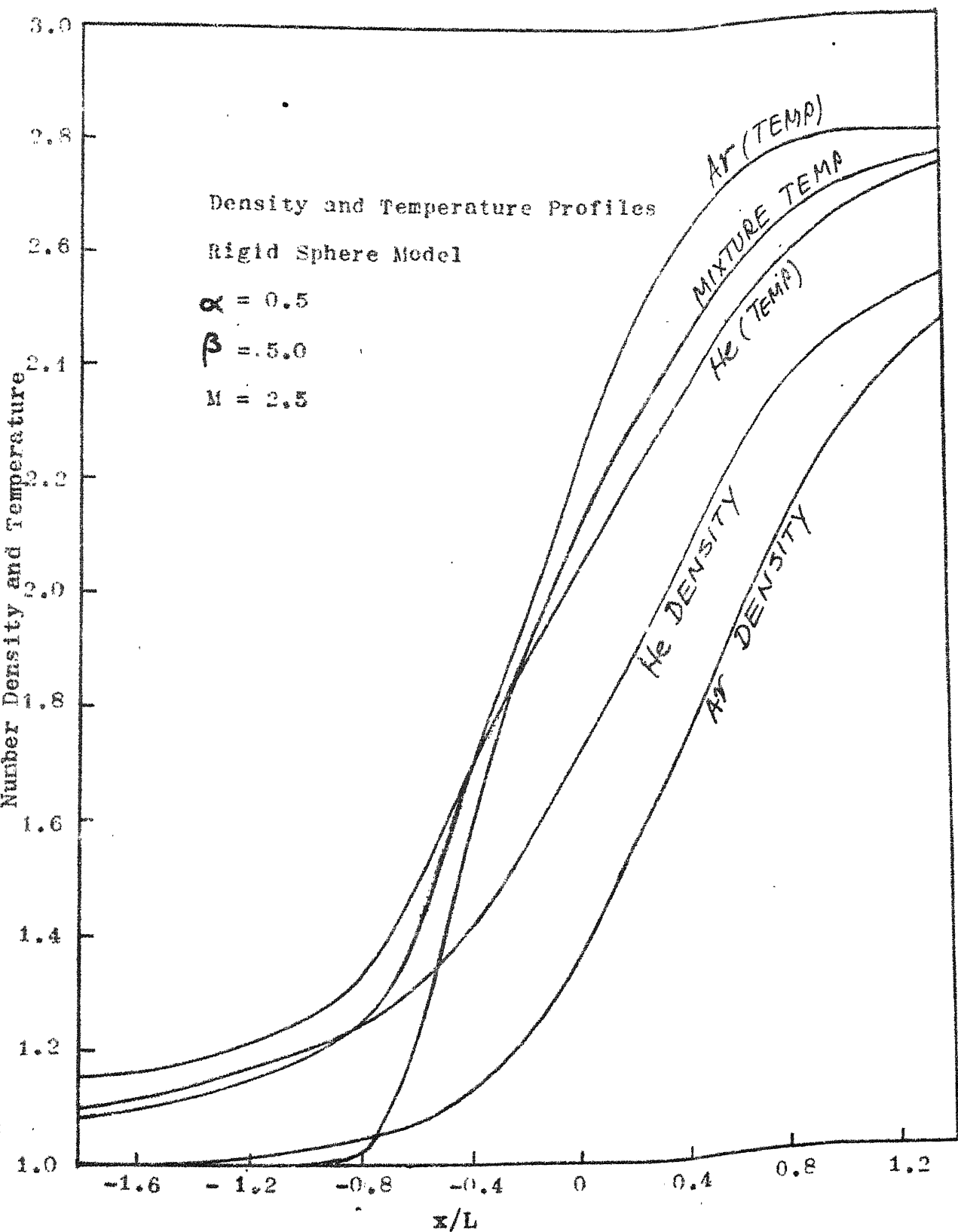
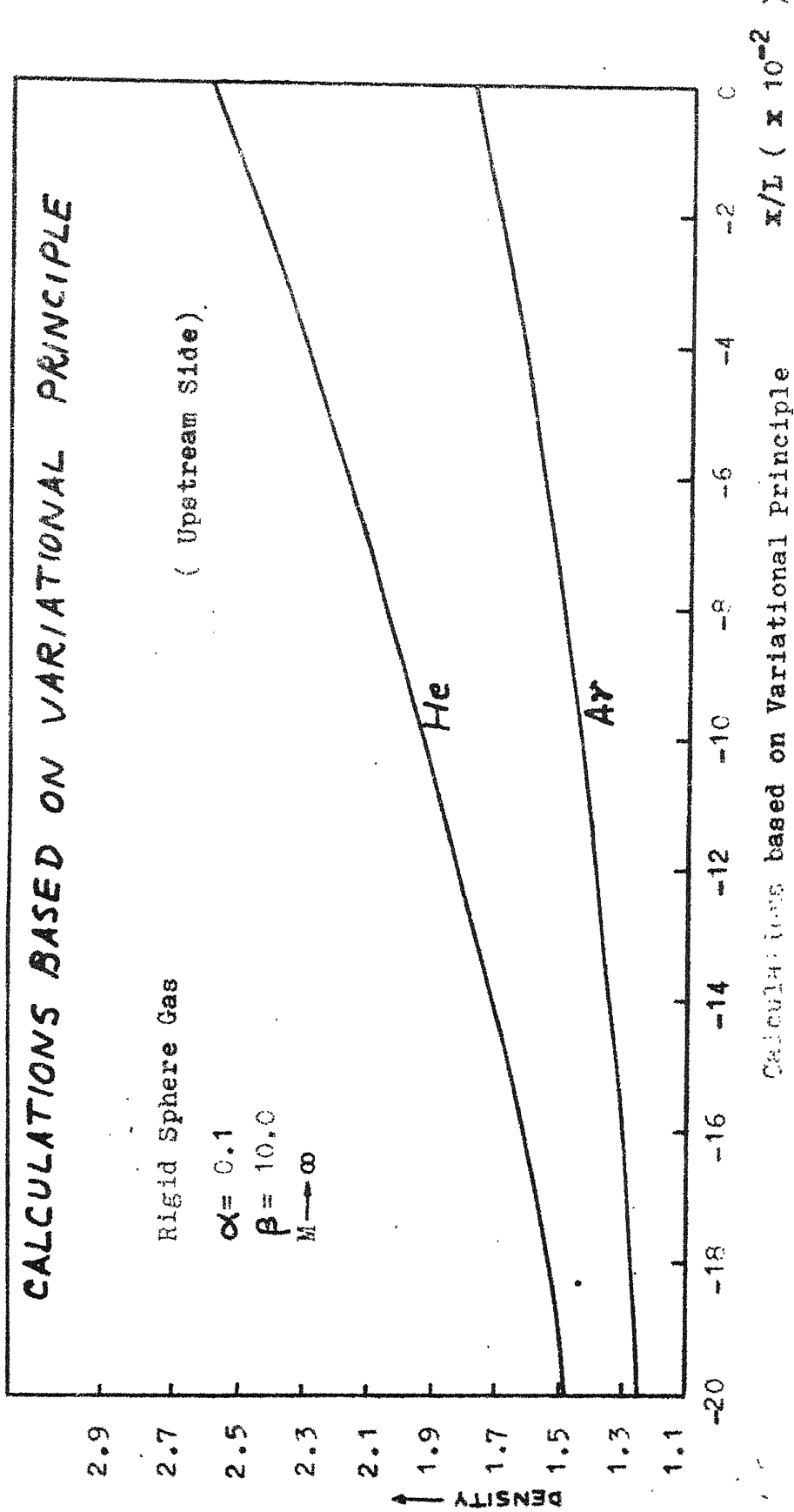
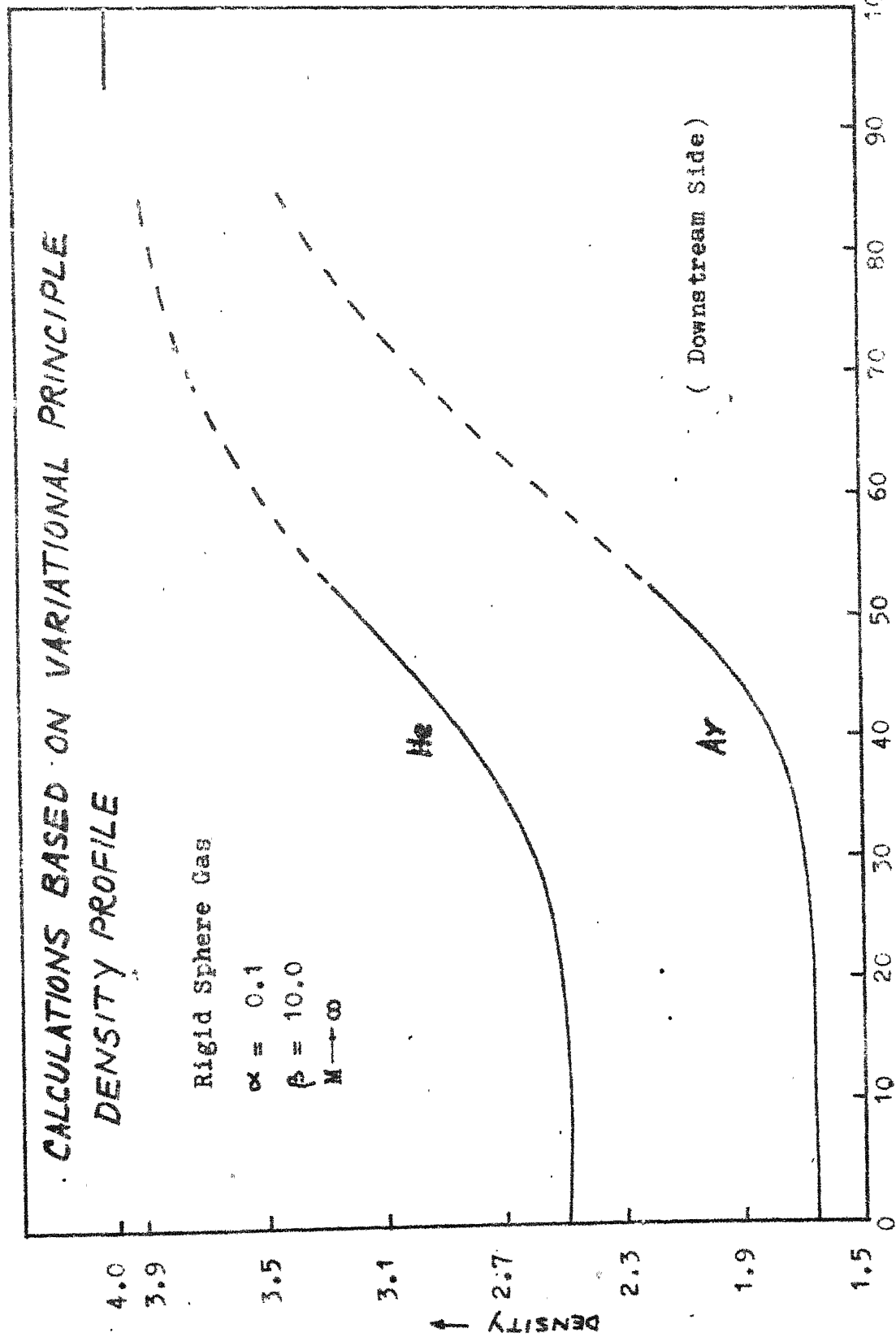


FIG 30 TEMPERATURE AND DENSITY PROFILES



**FIG 31(Q) DENSITY PROFILE**





Calculations based on Variational Principle

**FIG 31(b) DENSITY PROFILE**

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